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Extension of the Representative Elementary Watershed approach for cold regions via explicit treatment of energy related processes

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Abstract. The paper extends the Representative Elementary Watershed (REW) theory for cold regions through explicit treatment of energy balance equations to include associated processes and process descriptions. A new definition of REW is presented which subdivides the REW into six surface sub-regions and two subsurface sub-regions. Vegetation, snow, soil ice, and glacier ice are included in the system so that such phenomena as evaporation/transpiration, melting, freezing, and thawing can be modeled in a physically reasonable way. The sub-stream-network is separated from other sub-regions so that the sub-REW-scale runoff routing function can be modeled explicitly. The final system of 24 ordinary differential equations (ODEs) can meet the requirements of most hydrological modeling applications, and the formulation procedure is re-arranged so that further inclusion of sub-regions and substances could be done more easily. The number of unknowns is more than the number of equations, which leads to the indeterminate system. Complementary equations are provided based on geometric relationships and constitutive relationships that represent geomorphological and hydrological characteristics of a watershed. Reggiani et al. (1999, 2000, 2001) and Lee et al. (2005b) have previously proposed sets of closure relationships for unknown mass and momentum exchange fluxes. Tian (2006) has applied Lee's procedures and formulas and Monte Carlo simulation method, and has come up with a determinate system based on the equations, though precluding energy balance ones, proposed in this paper. The additional geometric and constitutive relationships required to close the new set of balance equations will be pursued in a subsequent paper.

1 Overview

The current generation of physically-based hydrological models, such as SHE (Abbott et al., 1986a, b), MIKE SHE (Refsgaard and Storm, 1995), IDHM (Beven et al., 1987; Calver and Wood, 1995), and GBHM (D. Yang et al., 2000, 2002a, b), is based on the point scale equations derived from Newtonian mechanics, as first set out by Freeze and Harlan (1969). These physically-based models have distinctive advantages over the so-called conceptual models that are based only on the mass balance principle. The hydrological literature is replete with reviews and discussions of the advantages and limitations of physically-based distributed models (Beven, 1989, 1993, 1996, 2002; Grayson et al., 1992; Smith et al., 1994; Woolhiser, 1996; Refsgaard et al., 1996; Singh and Woolhiser, 2002). The most important limitation is perhaps the mismatch between the scale at which the governing equations are applicable and the scale at which models are applied, and the associated difficulties due to the nonlinearity of equations and the heterogeneity of landscape properties. There are two complementary approaches to resolve the above problems. One is to devise new balance equations applicable directly at the spatial scale of a watershed, the scale at which most hydrological forecasts and predictions are required. The other is to devise effective parameters to account for the heterogeneity. The latter approach can be coupled either with the current small-scale governing equations or with the new equations developed at the scale of watersheds, as mentioned above. A number of approaches towards such parametrization have been proposed so far to be coupled with mostly conceptual models (Viney and Sivapalan, 2004; Robinson and Sivapalan, 1995; Duffy, 1996; Ewen, 1997). No concerted effort has been made, however, to develop the scale adaptable equations.

The Representative Elementary Watershed (REW) approach, originally outlined by Reggiani et al. (1998, 1999), is an ambitious attempt to invoke mass, momentum, and energy

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Table 1. Sub-regions and materials of a REW after Reggiani et al. (1998).

No.	sub-region	materials contained
1	saturated zone	water, soil matrix
2	unsaturated zone	water, gas, soil matrix
3	saturated overland flow zone	water
4	concentrated overland flow zone	water
5	main channel reach	water

balances and entropy constraints directly at the watershed scale (Beven, 2002). The REW approach treats a watershed as a continuous, open thermodynamic system with discrete sub-watersheds called Representative Elementary Watersheds (REWs), where the REW is deemed as the smallest elementary unit for hydrological modeling. The REW is further divided into several functional sub-regions (in Reggiani et al.'s formulation, there are five sub-regions, as discussed below in Sect. 2). REWs and sub-regions are sub-continua of the whole watershed hydrological system. The general conservation laws for mass, momentum, energy, and entropy are then applied to the entire system and to its sub-continua. The resulting ordinary differential equations (ODEs), after averaging over characteristic time and sub-region volume, can then be applied directly at the REW scale. Many researchers have developed initial closure relationships required by the REW approach and the resulting numerical models (Reggiani and Sivapalan, 2000; Reggiani et al., 2001; Reggiani and Rientjes, 2005; Lee et al., 2005a, b, 2006; Zhang and Savenije, 2005). The application of these closure schemes to hypothetical, experimental, and natural watersheds shows that the REW approach can indeed simulate and predict watershed hydrological response soundly and reasonably.

In spite of the rapid advances in theory and application, the REW approach, however, cannot presently take full and comprehensive account of evaporation/transpiration occurring on various land surfaces, and hydrological processes related with cold regions such as melting, freezing, and thawing, because of the restrictive definition of REW structure. In fact, the combined processes of evaporation and transpiration, which constitute total evaporation or sometimes are called evapotranspiration, are major components of the hydrological cycle (Ward and Robinson, 1990). It accounts for the disposal of over 90 percent of precipitation in arid regions, about 50–75 percent in humid regions and 60 percent globally, and occurs on open water surfaces, bare soil surfaces, vegetation surfaces, and leaf stomas. It is also the dominant variable in the land surface energy balance equation. Evapotranspiration, therefore, must be an elementary component of hydrological models which cannot be represented in a physically reasonable way in Reggiani's origi-

nal formulation (Reggiani et al., 1999). As for melting from snowpack and glaciers, it is often a crucial component of the hydrological cycle, especially in cold regions which cover nearly half of global land area (Z. Yang et al., 2000; Fassnacht, 2000) at least in some parts of the year. For example, in the western United States, approximately 75 percent of the total water budget comes from snowmelt (McManamon et al., 1993; Williams and Tarboton, 1999), and the north-western inland arid area of China relies heavily on melting snow and glaciers for its annual water supply (Z. Yang et al., 2000). Besides, due to the wide extent of frozen soil on the land surface (Z. Yang et al., 2000; Fassnacht, 2000), the release and uptake of energy through phase transition in the processes of freezing and thawing, and the resulting change of soil hydraulic and thermal properties, soil freezing and thawing have significant influences on local and global water and energy cycle (Hu et al., 2006). These important processes occurring in the immense cold regions which are intensively coupled with energy supply and transfer processes, however, cannot be modeled in Reggiani et al.'s (1998) original formulation at all. In order to serve as an alternative blueprint for hydrological modeling, therefore, the REW approach should be generalized to model these energy related processes occurring on various land surfaces in a physically reasonable way.

The purpose of this paper, then, is therefore to re-derive the REW scale balance equations by following Reggiani et al.'s (1998) procedure, but explicitly considering these energy related processes. We begin with a review of Reggiani et al.'s (1998) REW definition and their REW scale balance equations. We then present our new definition based on an expanded application of the concept of the REW. After introducing the symbols and notations related to the introduced variables, we use these to describe the geometric, kinetic, and thermodynamic properties of hierarchical continua. We then re-configure the general form of the balance equations for mass, momentum, energy, and entropy at the REW scale by applying the averaging method pioneered by Hassanizadeh and Gray (1979a, b, 1980). To confine the problem to understandable and manageable levels, a series of simplifying assumptions are then presented. Finally, a new set of ODEs is proposed. In order to facilitate the adoption of the new equations in hydrological modeling practice, the relevant geometric relationships need to be presented and improved. Likewise, the constitutive relationships for the new exchange terms for mass, momentum, and energy also need to be devised, and revised. While acknowledging that these are essential, their actual derivation will not be presented here; instead, they will be presented in a subsequent paper.

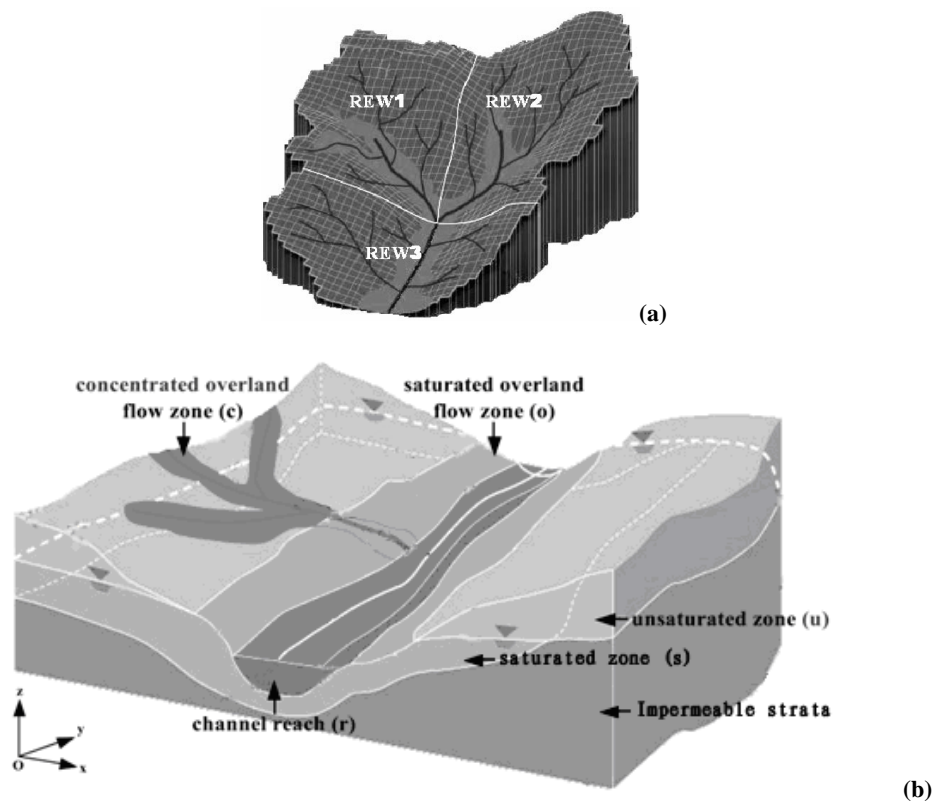


Fig. 1. (a) Catchment discretization into 3 REW units (b) Sub-regions making up the spatial domain of a REW (after Reggiani et al., 1998 and Lee et al., 2005b).

2 Review of the REW definition and REW scale balance equations by Reggiani et al. (1998, 1999)

From a hydrological perspective, a watershed and its hierarchical sub-watersheds present self-similar characteristics. We consider a sub-watershed as a fundamental component of hydrological modeling termed the Representative Elementary Watershed (REW). Reggiani et al. (1998) divide a watershed into REWs, and then further divide each REW into five sub-regions (see Fig. 1): saturated zone (s-zone), unsaturated zone (u-zone), saturated overland flow zone (o-zone), concentrated overland flow zone (c-zone), and main channel reach (r-zone). Table 1 shows all the sub-regions in a REW and their respective substances.

Based on the division of a catchment into elementary units (REWs) and sub-regions (zones), Reggiani et al. (1998) derived global balance laws for mass, momentum, energy, and entropy at the spatial scale of REW, which can represent various hydrological flow processes. However, being a first attempt, various energy related processes cannot be represented although the energy balance equations are indeed included in Reggiani et al.'s (1998) original formulation due to the limitations of their REW definitions:

- (1) Vegetation layer is excluded in the definition, and therefore, transpiration cannot be modeled physically. In Reggiani et al.'s (1998) formulation, transpiration is combined with evaporation and is deemed as a phase transition from liquid to vapor which occurs within the u-zone, i.e., the soil (Reggiani and Sivapalan, 2000; Reggiani and Rientjes, 2005; Lee et al., 2005b, 2006), which differs from the actual vaporization process occurring across leaf stomas.
- (2) Phases such as soil matrix, gas, and water are included in the definition, but phases such as snow, soil ice, and glacier ice are excluded. Hydrological phenomena such as accumulation and depletion of snow pack and glacier, and freezing and thawing of the soil ice are, therefore, excluded from consideration.
- (3) The fact that the land surface is divided into two different overland flow zones and the main channel reach does help to represent various flow processes conveniently (Reggiani et al., 1998), but still cannot represent evaporation/transpiration occurring from various kinds of land cover such as water, vegetation, bare soil, snow, and glacier.

Table 2. Structure of redefined REW (sub-regions).

No.	layer	sub-region	abbreviation
1	subsurface	unsaturated zone	u
2	subsurface	saturated zone	s
3	surface	main channel reach zone	r
4	surface	sub stream network zone	t
5	surface	bared zone	b
6	surface	vegetation covered zone	v
7	surface	snow covered zone	n
8	surface	glacier covered zone	g

Furthermore, Reggiani et al.'s definition of REW also exhibits the following limitations:

- (4) The way that the sub-REW-scale network of channels, rills and gullies is included in the c-zone is somewhat ambiguous. The sub-REW-scale network of channels, rills, gullies, as well as lakes, reservoirs, etc., namely, sub-stream-network, is water body, and its role in hydrological processes is distinct from that of the land surface. The sub-stream-network can serve as not only runoff generation areas but also as runoff routing pathways, and the latter function is by no means less important than the former one, especially in a REW with large area. We cannot represent the sub-REW-scale runoff routing function physically if the sub-stream-network is embedded in other sub-regions.

In summary, the REW approach in its present form cannot take fully into account energy related processes. In its current applications, therefore, energy balance equations are considered as identical equations and omitted due to the isothermal assumption (Reggiani et al., 1999), which especially precludes the application of the REW approach and associated models (Reggiani and Rientjes, 2005; Lee et al., 2006) in cold regions. Generalizing the REW theory to represent energy related processes, through an explicit inclusion of vegetation, snow, soil ice, and glacier into the REW definition, is the subject matter of this paper.

3 Redefinition of Representative Elementary Watershed

Owing to the limitations of the original REW definition discussed above, a new definition is proposed focusing on the re-configuration of REW's surface layers. Available data for modeling water movement beneath the land surface in detail is scarce in most of the natural watersheds. The subsurface layer, therefore, is separated from the surface layer and simply divided into a saturated zone and an unsaturated zone

with the water table as the interface, which is similar to Reggiani et al.'s work. For the surface layer, hillslopes and the channel network can be deemed as two fundamental components of a watershed. Therefore, the surface layer is divided into two sections—hillslope and stream network, just as Reggiani et al. had done. To account for the sub-REW-scale runoff routing function explicitly, the sub-stream-network, which is embedded into the c-zone in Reggiani et al.'s definition, coexists with the main channel reach in the stream network section in our new definition, and lakes, reservoirs, rills, and gullies are incorporated into the sub-stream-network in order to maintain scale invariability in the REW structure. Hillslopes, which are the primary regions for runoff generation as well as water dissipation, must be treated with by its flow nature and evaporation/transpiration nature simultaneously. Therefore, the original hillslope division scheme containing o-zone and c-zone, which is intended to account for various flow processes, is inadequate for hydrological modeling physically. In our new definition, the hillslope is divided into various kinds of land covers which presently include bare soil zone, vegetated zone, snow covered zone, and glacier covered zone.

In total, we defined two sub-regions in the subsurface layer and six sub-regions in the surface layer of a REW (see Table 2 and Fig. 2). By choosing a proper spatial scale according to data availability and simulation objective, a watershed can be divided into discrete REWs with unique soil types and hydrogeological conditions, vegetation categories, and snow and glacier cover characteristics, in a similar way that the SWAT model defines Hydrological Response Units (Arnold et al., 1998; Srinivasan et al., 1998). On the spatial side, the six surface sub-regions constitute a complete cover of the land surface in the horizontal direction. In the vertical direction, we assume the four sub-regions of bare soil, vegetated, snow covered, and glacier covered zones lie above the unsaturated zone. The other two surface sub-regions, i.e., the main channel reach and sub-stream-network may lie above either the saturated or unsaturated zone relative to their relationship to the water table.

For consideration of soil freezing and thawing, the ice phase is included in the subsurface sub-regions in addition to soil matrix, liquid water, and gas. For consideration of evaporation and transpiration, the vapor phase is included in all the surface sub-regions. For subsurface sub-regions, the unsaturated zone has also a vapor phase which coexists with air in the soil pores. We define the mixture of water vapor and air, therefore, as the gaseous phase for the unsaturated zone (and snow covered zone, as detailed below). For details about the materials associated with every sub-region, see Table 3, and for a summary of all the different materials involved in the REW, see Table 4.

We consider evaporation and transpiration to occur from the surface sub-regions only. In spite of the gaseous phase in the unsaturated zone, no evaporation is considered to occur in the subsurface layer since the vaporization of water within

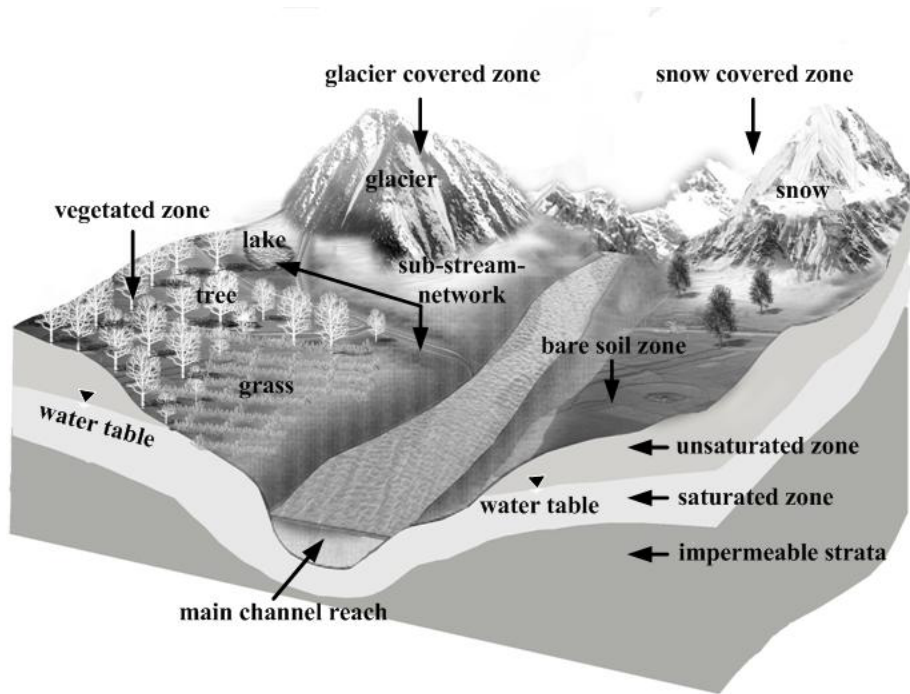


Fig. 2. Sub-regions of the redefined REW.

the soil is small compared with evaporation/transpiration occurring from various land surfaces (Jacobs et al., 1999). Whereas the vapor phase is included in each surface sub-region, it cannot be stored. The vapor phase disperses into the atmosphere immediately after its formation due to the phase transition from liquid water or ice. The snow covered zone is an exception to this rule. It includes snow, liquid water, and gas, and in this way it is similar to the porous media. The snow covered zone can contain liquid water to a certain degree as saturation content in the soil, and correspondingly can contain a limited gaseous phase.

Surface runoff can be generated on each surface sub-region when the intensity of rainfall exceeds the infiltration capacity of the sub-region. In our new definition, infiltration excess flow (Hortonian overland flow, also known as concentrated overland flow in Reggiani et al.'s formulation) is no longer separated from saturation excess flow (saturated overland flow) because their underlying unified mechanism (Rui, 2004). In fact, different types of runoff generation can occur only on the interface formed by media with different infiltration capacities, and the infiltration capacity of the upper medium must be higher than that of the lower medium. On such interfaces, runoff will be actually generated when the intensity of water supply to the interface (which cannot exceed the infiltration capacity of the upper medium) exceeds the infiltration capacity of the lower medium. Land surface, for example, is one of such interfaces, of which the upper medium is the atmosphere with infinite penetration capacity

Table 3. Materials contained in each sub-region.

No.	sub-region	materials	abbreviation
1	u-zone	soil m atrix	m
2	u-zone	l iquid water	l
3	u-zone	g as	a
4	u-zone	i ce	i
5	s-zone	soil m atrix	m
6	s-zone	l iquid water	l
7	s-zone	i ce	i
8	r-zone	l iquid water	l
9	r-zone	v apor	p
10	t-zone	l iquid water	l
11	t-zone	v apor	p
12	b-zone	soil m atrix	m
13	b-zone	l iquid water	l
14	b-zone	v apor	p
15	v-zone	v egetation	v
16	v-zone	l iquid water	l
17	v-zone	v apor	p
18	n-zone	s now	n
19	n-zone	l iquid water	l
20	n-zone	g as	a
21	g-zone	i ce	i
22	g-zone	l iquid water	l
23	g-zone	v apor	p

Table 4. All materials involved in REW.

No.	materials	abbreviation
1	soil matrix	m
2	liquid water	l
3	gas	a
4	vapor	p
5	ice	i
6	snow	n
7	vegetation	v

for water, and the lower medium is the unsaturated soil when infiltration excess flow occurs or the saturated soil when saturation excess flow occurs. Therefore, runoff generation can be modeled physically without the separation of infiltration excess flow and saturation excess flow.

Similarly, subsurface flow can be generated when the soil is heterogeneous in the unsaturated zone. For example, if the unsaturated zone is composed of two soil layers and the infiltration capacity of the top layer is greater than that of the lower layer, subsurface flow can be generated on the interface between the top and the lower layer. In Reggiani et al.’s definition, and even in our new definition of REW, such heterogeneity is excluded explicitly in order to avoid over-complexity, and the subsurface flow and associated preferred flow (Lei et al., 1999) are embedded in the mass exchange terms between the unsaturated zone and the neighboring REW or the external world, and taken into account by the corresponding constitutive relationships, as demonstrated by Lee et al. (2005b).

The water storage in the bare soil zone represents depression storage; the water storage in the vegetated zone represents canopy interception and also depression storage, whereas water cannot be stored in the glacier covered zone. In each case, the liquid water gathered from rainfall in the surface sub-regions, or transferred from ice in the glacier covered zone, or transferred from snow in the snow covered zone, flows into the sub-stream-network, and then into the main channel reach.

The six defined types of surface sub-regions can meet most of the requirements for watershed scale hydrological modeling. There is no doubt, however, that some special surface sub-regions will be needed in special situations. For example, reservoir and urbanized zones may be needed in order to incorporate human activities. Also, the composite zone of two or more basic types of land cover defined above, such as the composition of snow and vegetation, or the particular separation of different vegetation types may be needed for detailed simulation. Following the procedure proposed in later sections, fortunately, new sub-regions can easily be added to the existing REW system without violating the general form of the balance equations derived below, as demon-

strated in Appendix B. Certainly, new sub-regions will introduce new exchange terms of mass, momentum, and energy. These will require the specification of additional geometric and constitutive relationships for the closure and determinacy of the balance equations.

The sub-regions or zones are further described below.

Saturated zone (s-zone): Similar to Reggiani et al.’s definition, the saturated zone is delimited by the water table on the top and by a limit depth reaching into the groundwater reservoir or by the presence of an impermeable stratum at the bottom. Laterally the saturated and unsaturated zones are delimited by the mantle surfaces from the neighboring REWs or by the external watershed boundary.

The materials contained within the saturated zone are the soil matrix, liquid water, and ice. The soil matrix and ice form the skeleton for water movement and phase transition between liquid water and ice may result from natural energy processes.

Unsaturated zone (u-zone): The physical boundary of the unsaturated zone is defined by Reggiani et al. (1998) in detail. The materials contained within the unsaturated zone are the soil matrix, liquid water, gas, and ice. Mass exchange terms include infiltration from the land surface, recharge into or capillary rise from the saturated zone, thawing or freezing, and lateral inflow/outflow through the mantle surfaces.

The location and area/volume of u-zone/s-zone depend on the water table fluctuation, geomorphology, and hydrogeological characteristics. We can estimate the dynamic spatial extent (area/volume) of the unsaturated zone with the help of digital elevation model (DEM) and Geographic Information System (GIS) software, provided that the location of the dynamic water table could be specified or estimated. Such geometric relationships are pursued independently by both Reggiani and Rientjes (2005), and Lee et al. (2005b) in different ways, and can also be adopted in our new definitions.

Main channel reach (r-zone): The main channel reach receives water from the sub-stream-network and transfers it towards the watershed outlet. It also exchanges water with the saturated zone or unsaturated zone. Of all the surface sub-regions, this is the only zone which can exchange water, momentum with the neighboring REWs or the external world. The water course of the main channel reach can be determined either by field observation or by DEM analysis. The materials contained within the main channel reach are water and vapor.

Sub-stream-network zone (t-zone): The sub-stream-network zone is the areal volume occupied by lakes, reservoirs, and the sub-REW-scale network of channels, rills, gullies, and ephemeral streams. It gathers water from the hillslopes and transfers it into the main channel reach. Its storage capacity and flow velocity are of importance for

sub-REW-scale runoff routing. The substances contained within sub-stream-network are water and vapor.

The location and area of lakes, reservoirs, or other large water bodies can be determined by field or remote observation, and that of the sub-REW-scale network of channels etc. can be determined by field observation or DEM analysis, similar to the main channel reach.

Vegetated zone (v-zone): The vegetated zone is the volume occupied by vegetation which intercepts precipitation, extracts water from the unsaturated zone through the roots, and evaporates it into the atmosphere in the form of transpiration. The intercepted water will also be evaporated into the atmosphere, eventually. The water storage in this zone represents canopy interception storage and depression storage. The horizontal projected area of this zone changes with the calendar and the cultivation season which could be measured by remote observation or modeled by various crop models (Cong, 2003). The materials contained in the vegetated zone are vegetation, water, and vapor.

Snow covered zone (n-zone): The snow covered zone is the volume of snow pack which plays an important role in hydrology and in the energy cycle in cold regions. The location of the snow covered zone can easily be determined by field or remote observation. Its area and depth are key factors for hydrological modeling in cold regions. However, they cannot easily be recognized and much literature can be found about their measurement and modeling (Maurer et al., 2003; Chen et al., 1996; Cao and Liu, 2005), which is helpful towards the development of the corresponding constitutive relationships. The materials contained in the snow covered zone are snow, water, and gas.

Glacier covered zone (g-zone): The glacier covered zone is the volume occupied by glacier ice whose location is always fixed. The materials contained in this zone are ice, liquid water, and vapor.

Bare soil zone (b-zone): The bare soil zone is the volume occupied neither by vegetation, nor by snow, nor by glacier, nor by sub-stream-network, nor by main channel reach. The water storage of this zone represents the depression storage. The horizontal projected area varies with the area of other surface sub-regions. The substances contained in this zone are bare soil, liquid water, and vapor.

4 Geometric, kinetic, and thermodynamic properties of hierarchical continua

In the REW approach, the entire watershed system is constituted by a finite number M of discrete REWs. Each REW is then divided into two subsurface sub-regions and six surface sub-regions. Several materials are included within each sub-

region. In terms of thermodynamics, the watershed system is composed of three hierarchical subsystems.

- (1) REW level: every discrete REW is treated as a subsystem of the entire watershed system, which is called REW level subsystem. There are M discrete REW level subsystems in a watershed made up of M REWs;
- (2) Sub-region level: every sub-region in a REW is treated as a subsystem of the REW level thermodynamic system, which is called sub-region level subsystem. There are eight sub-region level subsystems in one REW level system;
- (3) Phase level: every type of substance in a sub-region is treated as a subsystem of a sub-region level thermodynamic system, which is called phase-level subsystem. The number of phase level subsystems included in a sub-region level system can be seen in Table 3, and there are in all 23 phase level subsystems in one REW level system.

We can thus regard the watershed, the REWs, the sub-regions, and the phases as hierarchical continua from a continuous mechanics perspective. Before applying conservation laws for subsystems or the continua as defined above, we will describe in turn the geometric, kinetic, and thermodynamic properties at the REW level, sub-region level, and phase level, following on from Reggiani et al. (1998), but proposed here in a more systematic and consistent manner.

4.1 Geometric description of the REW level continuum

The number of discrete REWs in a watershed is denoted by M . The k^{th} REW is marked by $B(K)$, $K \in \{e | e=1..M\}$, where B indicates the body of a continuum. The number of REWs neighboring $B(K)$ is denoted by N_K . The space occupied by all the materials contained within $B(K)$ is denoted by $V(K)$ where $V(K)$ is a prismatic volume (for details the reader should refer to Reggiani et al., 1998).

The surface of the prism is recorded as $S(K)$ which includes the following components:

- (1) Side surfaces: the side surface of $B(K)$ can be divided into a series of segments, of which the segment formed by the interfaces between $B(K)$ and $B(L)$ ($L=1..N_K$) is denoted by $S^L(K)$, the segment formed by the interfaces between $B(K)$ and the external world is denoted by $S^{EXT}(K)$.
- (2) Top surface: the top surface of $B(K)$ formed by the interface between the atmosphere and the land surface covering $B(K)$ is an irregular curved surface which is denoted by $S^T(K)$. The projection of $S^T(K)$ onto the horizontal plane is denoted by $\sum(K)$, and the contour of $S^T(K)$ is denoted by $C(K)$.

- (3) Bottom surface: the bottom surface of $B(K)$, denoted by $S^B(K)$, is the impermeable strata or a hypothetical plane at a given depth reaching into the groundwater reservoir or the combination of the two.

4.2 Geometric description of the sub-region level continuum

The sub-region level continua divided from $B(K)$ and the phase level continua included in a sub-region are denoted by $B^j(K)$ and $B_\alpha^j(K)$, respectively, where $j \in \{e|e=u, s, r, t, b, v, n, g\}$, $\alpha \in \{\zeta|\zeta=m, l, a, p, i, n, v\}$ (see Table 3). The volumes occupied by $B^j(K)$, $B_\alpha^j(K)$ are denoted by $V^j(K)$, $V_\alpha^j(K)$, respectively. $B^s(K)$ (the saturated zone) and $B^u(K)$ (the unsaturated zone) occupy a 3-D space, while $B^r(K)$ (the main channel reach) is linear, while the other zones are planar.

$B^j(K)$ exchanges mass, momentum, and energy with environment through its interface $S^j(K)$, which can be divided into the following components:

- (1) Interface between $B^j(K)$ and the external world, which is denoted by $S^{jEXT}(K)$.
- (2) Interface between $B^j(K)$ and $B(L)$ ($L=1..N_K$), which is denoted by $S^{jL}(K)$.
- (3) Interface between $B^j(K)$ and the atmosphere on the top, which is denoted by $S^{jT}(K)$.
- (4) Interface between $B^j(K)$ and the impermeable strata or groundwater reservoir at the bottom, which is denoted by $S^{jB}(K)$.
- (5) Interface between $B^j(K)$ and $B^i(K)$ ($i \neq j$), the other sub-regions within the same REW, which is denoted by $S^{ji}(K)$, ($i \neq j$).

In our derivation, we use dS to denote the differential area vector of the surface. For the surfaces discussed above, the corresponding differential area vector symbols, $dS^{jEXT}(K)$, $dS^{jL}(K)$, $dS^{jT}(K)$, $dS^{jB}(K)$, and $dS^{ji}(K)$, are defined. These differential vectors point to the side indicated by the second superscript from the side indicated by the first superscript along the normal direction of the differential area, and the following equations hold

$$\left. \begin{aligned} S^{ji} &= S^{ij} \\ dS^{ji} &= -dS^{ij} \end{aligned} \right\} j \neq i. \quad (1)$$

We also define the area vector for interface S^{jP} using the wildcard P as

$$S^{jP} = \int_{S^{jP}} dS^{jP}, P=EXT, L, T, B, i, L=1..N_K, i \neq j. \quad (2)$$

4.3 Definition of the time-averaged REW-scale quantities

To formulate the balance equations at the macro scale of both time and space, the geometric, kinetic, and thermodynamic quantities should be averaged, as Reggiani et al. (1998) originally defined. For consistency we rewrite these definitions below.

In the following sections, the identifier of individual REW, K , is omitted in the interest of brevity unless confusion arises in which case it is included.

Definition 1: The fraction of time-averaged horizontal projected area of B^j in Σ , $j \neq r$

$$\omega^j = \frac{1}{2\Delta t \Sigma} \int_{t-\Delta t}^{t+\Delta t} \Sigma^j(\tau) d\tau, j \neq r, \quad (3)$$

where $2\Delta t$ is the time interval, Σ is the horizontal projected area of $B(K)$, Σ^j is the horizontal projected area of B^j .

Definition 2: The time-averaged thickness of B^j , $j \neq r$

$$y^j = \frac{1}{2\Delta t \omega^j \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{V^j} dV d\tau, j \neq r \quad (4)$$

Definition 3: The time-averaged volume fraction of B_α^j relative to V^j , $j \neq r$

$$\varepsilon_\alpha^j = \frac{1}{2\Delta t y^j \omega^j \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{V^j} \gamma_\alpha^j dV d\tau, j \neq r \quad (5)$$

where γ_α^j is the phase distribution function on α phase in j sub-region, see Definition 10 below for detail.

Definition 4: The time-averaged density of B_α^j , $j \neq r$

$$\bar{\rho}_\alpha^j = \frac{1}{2\Delta t \varepsilon_\alpha^j y^j \omega^j \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{V^j} \rho_\alpha^j \gamma_\alpha^j dV d\tau, j \neq r \quad (6)$$

where ρ_α^j is the density of α phase at the differential volume dV in V_α^j space.

Definition 5: The time-averaged physical quantity ϕ possessed by B_α^j relative to the mass of B_α^j , $j \neq r$

$$\bar{\psi}_\alpha^j = \frac{1}{2\Delta t \bar{\rho}_\alpha^j \varepsilon_\alpha^j y^j \omega^j \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{V^j} \rho_\alpha^j \psi_\alpha^j \gamma_\alpha^j dV d\tau, j \neq r \quad (7)$$

Definition 6: The time-averaged length of the main channel reach relative to Σ

$$\xi^r = \frac{1}{2\Delta t \Sigma} \int_{t-\Delta t}^{t+\Delta t} l^r d\tau, \quad (8)$$

where l^r is the instantaneous length of the main channel reach. It is constant in most cases, and ξ^r is, therefore, constant too.

Definition 7: The time-averaged cross section area of the main channel reach

$$m^r = \frac{1}{2\Delta t \xi^r \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{V^r} dV d\tau \quad (9)$$

Definition 8: The time-averaged density of B_α^r

$$\overline{\rho_\alpha^r} = \frac{1}{2\Delta t m^r \xi^j \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{V^r} \rho_\alpha^r \gamma_a^r dV d\tau, \quad (10)$$

where ρ_α^r is the density of α phase at the differential volume dV in V_α^r space.

Definition 9: The time-averaged physical quantity ϕ possessed by B_α^j relative to the mass of B_α^j , $j \neq r$

$$\overline{\psi_\alpha^r} = \frac{1}{2\Delta t \overline{\rho_\alpha^r} m^r \xi^r \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{V^r} \rho_\alpha^r \psi_a^r \gamma_a^r dV d\tau. \quad (11)$$

4.4 Geometric description of the phase level continuum

We introduce the definition of the phase distribution function in order to define physical quantities for the phase level continuum conveniently.

Definition 10: The phase distribution function of α phase substance in j zone showing the distribution of α phase in space V^j

$$\gamma_\alpha^j(dV) = \begin{cases} 1, & dV \in V_\alpha^j \\ 0, & dV \notin V_\alpha^j \end{cases} \quad (12)$$

The physical quantities defined in V_α^j space can be alternatively defined in V^j space by means of phase distribution function. This is also true for the physical quantity defined over the interface S_α^j . Therefore, through the use of the phase distribution function, we can omit the definitions of V_α^j and S_α^j , and focus on the phase interfaces between B_α^j and B_β^j ($\beta \neq \alpha$) within one sub-region, which is denoted by $S_{\alpha\beta}^j$, $\beta \neq \alpha$. Similarly, the symbol $dS_{\alpha\beta}^j$ is used for indicating the differential area vector of interface $S_{\alpha\beta}^j$, $\beta \neq \alpha$. It points to β phase from α phase along the normal direction of the differential area, and the following equations denote if:

$$S_{\alpha\beta}^j = S_{\beta\alpha}^j \quad dS_{\alpha\beta}^j = -dS_{\beta\alpha}^j, \quad \beta \neq \alpha. \quad (13)$$

We also define the area vector of interface $S_{\alpha\beta}^j$, $\beta \neq \alpha$ as

$$S_{\alpha\beta}^j = \int_{S_{\alpha\beta}^j} dS_{\alpha\beta}^j, \quad \beta \neq \alpha \quad (14)$$

4.5 REW-scale mass exchange terms through interfaces

Mass exchange terms through interfaces are the most important variables in a hydrological system. The definitions of time-averaged values of various REW-scale mass exchange terms relative to Σ , according to Reggiani et al. (1998), is given here for later use.

Definition 11: The net flux of α phase through S^{jP}

$$\begin{aligned} e_\alpha^{jP} &= \frac{1}{2\Delta t \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{S^{jP}} \rho_\alpha^j (\mathbf{w}_\alpha^j - \mathbf{v}_\alpha^j) \cdot \gamma_a^j dA d\tau, P \\ &= EXT, L, T, B, i, L=1..N_K, i \neq j, \end{aligned} \quad (15)$$

where \mathbf{v}_α^j is the velocity of the continuum B_α^j , \mathbf{w}_α^{jP} is the velocity of the interface S_α^{jP} .

Definition 12: The phase transition rate between α phase and β phase

$$e_{\alpha\beta}^j = \frac{1}{2\Delta t \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{S_{\alpha\beta}^j} \rho_\alpha^j (\mathbf{w}_{\alpha\beta}^j - \mathbf{v}_\alpha^j) \cdot \gamma_a^j dA d\tau \quad (16)$$

5 General form of the conservation laws and their averaging

5.1 General form of the conservation laws

In the REW approach, the derivations of the balance equations are based on the global conservation laws written in term of a generic thermodynamic property ψ . The averaging method developed by Hassanizadeh et al. (1979a, b, 1980, 1986a, b) and pioneered by Reggiani et al. (1998, 1999) is then applied.

Suppose a control volume V^* and its boundary surface is $A^* = \partial V^*$. At a specific time, the substances contained in V^* form a continuum B . For a conserved physical quantity ψ , the Euler description of its global generic conservation law is:

$$\begin{aligned} \frac{\partial}{\partial t} \int_{V^*} \rho \psi dV + \int_{A^*} \rho \psi (\mathbf{v} - \mathbf{w}) \cdot d\mathbf{A} \\ - \int_{A^*} \mathbf{i} \cdot d\mathbf{A} - \int_{V^*} (\rho f + G) dV = 0, \end{aligned} \quad (17)$$

where ρ is the mass density of the continuum, dV is the differential volume, dA is the differential area of the interface, $d\mathbf{A}$ is the differential area vector of the interface whose value is dA , direction is the normal direction pointing outward, \mathbf{v} is the velocity of a continuum, \mathbf{w} is the velocity of a continuum interface, ψ is the specific physical quantity ϕ with mass, \mathbf{i} is the diffusion flux, f is the source or sink term per unit mass, G is the source or sink term per unit volume. The quantities \mathbf{i} , f and G have to be chosen depending on the type of physical quantity ϕ that is considered (see Table 5 for detail).

5.2 General form of the time averaged conservation laws on the spatial scale of REW

Applying Eq. (17) to a phase level continuum B_α^j yields

$$\begin{aligned} \frac{\partial}{\partial t} \int_{V_\alpha^j} \rho_\alpha^j \psi_\alpha^j dV \\ + \sum_{P=EXT, L, T, B, i}^{L=1..N_K, i \neq j} \int_{S^{jP}} \rho_\alpha^j \psi_\alpha^j (\mathbf{v}_\alpha^j - \mathbf{w}_\alpha^{jP}) \cdot \gamma_a^j dA \\ + \sum_{\beta \neq \alpha} \int_{S_{\alpha\beta}^j} \rho_\alpha^j \psi_\alpha^j (\mathbf{v}_\alpha^j - \mathbf{w}_{\alpha\beta}^j) \cdot d\mathbf{A} \end{aligned}$$

Table 5. Summary of the properties in the conservation equation (after Reggiani et al., 1998).

Quantity	ψ	i	f	G
Mass	1	0	0	0
Linear Momentum	\mathbf{v}	\mathbf{t}	\mathbf{g}	0
Energy	$E+1/2v^2$	$\mathbf{t} \cdot \mathbf{v} + \mathbf{q}$	$h + \mathbf{g} \cdot \mathbf{v}$	0
Entropy	η	\mathbf{j}	b	L

Note: Where, \mathbf{t} is the microscopic stress tensor, \mathbf{g} is the gravity acceleration vector, E is the microscopic internal energy per unit mass, \mathbf{q} is the microscopic heat flux vector, h is the supply of internal energy from outside world, η is the microscopic entropy per unit mass, \mathbf{j} is the non-convective flux of entropy, b is the entropy supply from the external world, L is the entropy production within the continuum.

$$\begin{aligned}
& - \sum_{P=EXT, L, T, B, i}^{L=1..N_K, i \neq j} \int_{S^{jP}} \mathbf{i} \cdot \gamma_{\alpha}^j d\mathbf{A} - \sum_{\beta \neq \alpha} \int_{S_{\alpha\beta}^j} \mathbf{i} \cdot d\mathbf{A} \\
& - \int_{V_{\alpha}^j} (\rho_{\alpha}^j f + G) dV = 0
\end{aligned} \quad (18)$$

All the variables are defined based on the differential volume of the continuum or differential area of the interface. In other words, they are all the microscopic quantities which exhibit a mismatch with the macroscopic quantities required for watershed hydrological modeling. An averaging procedure in both time and space is necessary for obtaining balance equations directly at the spatial scale of the REW. This procedure has been pursued in detail in the Appendix A. In this section only the final results are presented. All the equations take the general form against a phase level continuum.

5.2.1 General form of mass conservation equation

$$\frac{d}{dt} (\overline{\rho_{\alpha}^j \varepsilon_{\alpha}^j y^j \omega^j}) = \sum_{P=EXT, L, T, B, i}^{L=1..N_K, i \neq j} e_{\alpha}^{jP} + \sum_{\beta \neq \alpha} e_{\alpha\beta}^j \quad (19)$$

5.2.2 General form of momentum conservation equation

$$\begin{aligned}
& \left(\overline{\rho_{\alpha}^j \varepsilon_{\alpha}^j y^j \omega^j} \right) \frac{d}{dt} (\overline{\mathbf{v}_{\alpha}^j}) \\
& = \overline{\mathbf{g}_{\alpha}^j \rho_{\alpha}^j \varepsilon_{\alpha}^j y^j \omega^j} + \sum_{P=EXT, L, T, B, i}^{L=1..N_K, i \neq j} \mathbf{T}_{\alpha}^{jP} + \sum_{\beta \neq \alpha} \mathbf{T}_{\alpha\beta}^j, \quad (20)
\end{aligned}$$

where the term on the l.h.s. is the inertial term, the first term on the r.h.s. is the weight of water. The remaining terms on the r.h.s. represent the various forces acting on the various interfaces, $\overline{\mathbf{v}_{\alpha}^j}$ is the velocity vector of the α phase averaged over the j sub-region, and $\overline{\mathbf{g}_{\alpha}^j}$ is the averaged gravity vector.

5.2.3 General form of heat balance equation

In Appendix A we present the conservation equation for mechanical energy and internal energy which is similar with Reggiani et al. (1998). We also derive the heat balance equation, with the additional terms due to velocity and internal energy fluctuation being ignored. The following heat balance equation is used in hydrological modeling:

$$\begin{aligned}
& \left(\overline{\varepsilon_{\alpha}^j y^j \omega^j c_{\alpha}^j} \right) \frac{d\overline{\theta_{\alpha}^j}}{dt} = \overline{h_{\alpha}^j \rho_{\alpha}^j \varepsilon_{\alpha}^j y^j \omega^j} \\
& + \sum_{P=EXT, L, T, B, i}^{L=1..N_K, i \neq j} Q_{\alpha}^{jP} + \sum_{\beta \neq \alpha} Q_{\alpha\beta}^j, \quad (21)
\end{aligned}$$

where on the l.h.s. the term represents the derivation of heat storage of α phase in j zone due to the variation of the temperature, on the r.h.s. the first term accounts for heat generation rate of α phase in j zone, the second term represents heat transfer rate from j zone to its environment, and the third term accounts for the heat transfer rate from α phase to the remaining phases within j zone, c_{α}^j is the specific heat capacity at a constant volume of α phase, $\overline{\theta_{\alpha}^j}$ is the temperature of α phase averaged over V_{α}^j , h_{α}^j is heat generation rate per unit mass in V_{α}^j , Q_{α}^{jP} is the rate of heat transferred from P zone to j zone, and $Q_{\alpha\beta}^j$ is the rate of heat transferred from β phase to α phase within j zone.

5.2.4 General form of entropy balance equation

$$\begin{aligned}
& \left(\overline{\rho_{\alpha}^j \varepsilon_{\alpha}^j y^j \omega^j} \right) \frac{d\overline{\eta_{\alpha}^j}}{dt} = \overline{b_{\alpha}^j \rho_{\alpha}^j \varepsilon_{\alpha}^j y^j \omega^j} \\
& + \overline{L_{\alpha}^j \rho_{\alpha}^j \varepsilon_{\alpha}^j y^j \omega^j} \\
& + \sum_{P=EXT, L, T, B, i}^{L=1..N_K, i \neq j} F_{\alpha}^{jP} + \sum_{\beta \neq \alpha} F_{\alpha\beta}^j, \quad (22)
\end{aligned}$$

where on the l.h.s. the term accounts for the derivation of entropy storage, on the r.h.s. the first term represents the supply rate of entropy from the external world, the second term is the internal entropy production rate within the subsystem, and the remaining terms are the various exchange terms across various interfaces.

6 Simplification of the equation sets

In previous sections, we have obtained the general form of the time-averaged conservation equations for mass, momentum, energy, and entropy against a phase-level continuum. In this section, we make a series of assumptions to keep the problem clearer and manageable, while meeting the requirements of hydrological modeling at the watershed scale. Then the interfaces across which the physical quantities such as

mass, momentum, energy, and entropy exchange are defined according to the assumptions. Finally, the general form of the averaged conservation laws is applied to each phase level continuum and their final balance equations obtained.

6.1 Assumptions for hydrological modeling in the REW approach

Assumption 1: Evaporation occurs from the surface sub-regions only.

Assumption 2: Vapor storage capacity and its velocity can be ignored in all sub-continua.

Assumption 3: Ice is static and rigid.

Assumption 4: Soil matrix is static, rigid, and inertial.

Assumption 5: All substances within the same sub-region possess the same temperature, and all surface sub-regions besides snow covered and glacier covered zones possess the same temperature, which is denoted by Θ^{surf} .

Assumption 6: Heat transfer occurs along the vertical direction only.

In above assumptions, Assumption 2, Assumption 3, and Assumption 4 are similar with the original ones (Reggiani et al., 1999), while Reggiani et al.'s (1999) assumption of an isothermal system is abandoned. This enables the equations developed here to simulate the energy related processes. Owing to the above assumptions, we can omit the following equations and mass exchange terms in the final results:

- (1) Balance equations of mass, momentum, and energy for gaseous substances, including gas and vapor;
- (2) Balance equations of mass, momentum, and energy for soil matrix;
- (3) Balance equation of momentum for soil ice;
- (4) Phase transition terms between gaseous phase and the remaining phases within u-zone;
- (5) Mass exchange terms between sub-regions are non-zero for the water phase only.

To be added, the exception for the last rule is the mass exchange term, e_g^{jT} , between j sub-region and atmosphere. However, the atmosphere is not a sub-region of the hydrological system but represents its external environment.

Table 6. Summary of the interfaces for each sub-region.

No	Sub-region	Interfaces
1	s-zone	$S^{sB}, S^{sEXT}, S^{sL}, S^{su}, S^{sr}, S^{st}, S_{li}^s$
2	u-zone	$S^{us}, S^{uEXT}, S^{uL}, S^{ub}, S^{uv}, S^{ug}, S^{un}, S_{li}^u$
3	b-zone	$S^{bT}, S^{br}, S^{bu}, S_{lp}^b$
4	v-zone	$S^{vT}, S^{vr}, S^{vu}, S_{lp}^v$
5	n-zone	$S^{nT}, S^{nr}, S^{nu}, S_{lp}^n$
6	g-zone	$S^{gT}, S^{gr}, S^{gu}, S_{lp}^g$
7	r-zone	$S^{rT}, S^{rEXT}, S^{rL}, S^{rt}, S^{rs}, S_{lp}^r$
8	t-zone	$S^{tT}, S^{tb}, S^{tv}, S^{tn}, S^{tg}, S^{tr}, S^{ts}, S_{lp}^t$

6.2 Interfaces in REW approach

Interfaces delimiting the watershed, REWs, sub-regions and phases determine the exchange terms arising in the balance equations. According to the above assumptions, interfaces in the REW approach are summarized in Table 6. For details about the symbols the reader should refer to the previous sections, especially Sect. 4, or the Nomenclature.

6.3 Balance equations for saturated zone

Substitution of mass, momentum, and energy exchange terms occurring within the saturated zone in Eq. (19), Eq. (20), and Eq. (21) with the help of the above assumptions leads to various conservation equations as follows:

6.3.1 Balance equation of mass for water phase

$$\frac{d}{dt} \left(\overline{\rho_l^s} \varepsilon_l^s y^s \omega^s \right) = e_l^{sEXT} + \sum_{L=1}^{N_K} e_l^{sL} + e_l^{sB} + e_l^{su} + e_l^{st} + e_l^{sr} + e_{li}^s \quad (23)$$

where the l.h.s. term accounts for the rate of change of water storage, the terms on the r.h.s. are various water exchange rate terms with the external world of the watershed, neighboring REWs, groundwater reservoir, u-zone, t-zone, r-zone, and ice phase, respectively.

From a hydrological perspective, the first two terms on the r.h.s of Eq. (23) represent the groundwater flow. e_l^{sB} accounts for the water exchange rate with deep groundwater, and it is zero when the bottom is impermeable. e_l^{su} represents water recharge term from u-zone into s-zone when it is positive, and capillary rise term from s-zone into u-zone when it is negative. e_{li}^s accounts for ice thawing term when it is positive, and water freezing term when it is negative.

6.3.2 Balance equation of mass for ice

$$\frac{d}{dt} (\overline{\rho_i^s \varepsilon_i^s y^s \omega^s}) = e_{il}^s = -e_{li}^s \quad (24)$$

6.3.3 Balance equation of momentum for water

$$\begin{aligned} & \overline{\rho_l^s \varepsilon_l^s y^s \omega^s} \frac{d}{dt} \overline{\mathbf{v}_l^s} - \overline{\mathbf{g}_l^s \rho_l^s \varepsilon_l^s y^s \omega^s} \\ & = \mathbf{T}_l^{sEXT} + \sum_{L=1}^{N_K} \mathbf{T}_l^{sL} + \mathbf{T}_l^{sB} + \mathbf{T}_l^{su} + \mathbf{T}_l^{st} + \mathbf{T}_l^{sr} + \mathbf{T}_{lm}^s + \mathbf{T}_{li}^s \end{aligned} \quad (25)$$

where the terms on the l.h.s. are the inertial term and weight of water, respectively. The r.h.s. terms represent various forces: the total pressure forces acting on the mantle segments in common with the external watershed boundary and neighboring REWs, the forces exchanged with the groundwater reservoir, the forces transmitted to u-zone across the water table, to t-zone across the seepage face, to r-zone across the seepage face, and the resultant forces exchanged with the soil matrix and the ice on the water-soil matrix and water-ice interfaces, respectively.

Owing to the Assumption 3 and Assumption 4, we can combine ice and the soil matrix together for momentum exchange. Therefore, the momentum terms of \mathbf{T}_{lm}^s and \mathbf{T}_{li}^s can be united into one single term $\mathbf{T}_{l(m,i)}^s$ which is denoted by \mathbf{T}_{lm}^s unless otherwise confusion would arise.

$$\begin{aligned} & \overline{\rho_l^s \varepsilon_l^s y^s \omega^s} \frac{d}{dt} \overline{\mathbf{v}_l^s} - \overline{\mathbf{g}_l^s \rho_l^s \varepsilon_l^s y^s \omega^s} \\ & = \mathbf{T}_l^{sEXT} + \sum_{L=1}^{N_K} \mathbf{T}_l^{sL} + \mathbf{T}_l^{sB} + \mathbf{T}_l^{su} + \mathbf{T}_l^{st} + \mathbf{T}_l^{sr} + \mathbf{T}_{lm}^s \end{aligned} \quad (26)$$

6.3.4 Balance equation of heat for water

$$\begin{aligned} & \varepsilon_l^s y^s \omega^s c_l^s \frac{d}{dt} \overline{\theta_l^s} - \lambda_l l_{il} e_{il}^s \\ & = \kappa_l^{sB} Q^{sB} + \kappa_l^{su} Q^{su} + \kappa_l^{st} Q^{st} + \kappa_l^{sr} Q^{sr}, \end{aligned} \quad (27)$$

where on the l.h.s. the first term represents the rate of change of heat storage due to variation of the temperature, and the second term represents heat of freezing. The terms on the r.h.s. are REW-scale heat exchange terms of water with the groundwater reservoir, u-zone, t-zone, r-zone, respectively, c_l^s is the specific heat capacity of water in s-zone at a constant volume, l_{il} is the latent heat of freezing, λ_l is the ratio of freezing heat absorbed by water, κ_l^{sB} is the ratio of the heat exchange term (across interface between s-zone and groundwater reservoir) absorbed by water, and κ_l^{su} , κ_l^{st} , κ_l^{sr} is the ratio of corresponding heat exchange term similarly absorbed by water.

6.3.5 Balance equation of heat for ice

$$\begin{aligned} & \varepsilon_i^s y^s \omega^s c_i^s \frac{d}{dt} \overline{\theta_i^s} - \lambda_i l_{il} e_{il}^s \\ & = \kappa_i^{sB} Q^{sB} + \kappa_i^{su} Q^{su} + \kappa_i^{st} Q^{st} + \kappa_i^{sr} Q^{sr}, \end{aligned} \quad (28)$$

where, similar to Eq. (27), λ_i is the ratio of freezing heat absorbed by ice, κ_i^{sB} is the ratio of heat exchange term (across interface between s-zone and groundwater reservoir) absorbed by ice, and κ_i^{su} , κ_i^{st} , κ_i^{sr} is the ratio of corresponding heat exchange term absorbed by ice.

6.3.6 Balance equation of heat for soil matrix

$$\begin{aligned} & \varepsilon_m^s y^s \omega^s c_m^s \frac{d}{dt} \overline{\theta_m^s} - \lambda_m l_{il} e_{il}^s \\ & = \kappa_m^{sB} Q^{sB} + \kappa_m^{su} Q^{su} + \kappa_m^{st} Q^{st} + \kappa_m^{sr} Q^{sr}, \end{aligned} \quad (29)$$

where λ_m is the ratio of freezing heat absorbed by the soil matrix, the meaning of other symbols is similar to those of Eq. (27) and Eq. (28).

The sum of the fraction of heat exchange terms absorbed by water, ice, and the soil matrix should be one, i.e.

$$\begin{aligned} & \kappa_l^{sB} + \kappa_i^{sB} + \kappa_m^{sB} = 1 \\ & \kappa_l^{su} + \kappa_i^{su} + \kappa_m^{su} = 1 \\ & \kappa_l^{st} + \kappa_i^{st} + \kappa_m^{st} = 1 \\ & \kappa_l^{sr} + \kappa_i^{sr} + \kappa_m^{sr} = 1 \\ & \lambda_l + \lambda_i + \lambda_m = 1 \end{aligned} \quad (30)$$

The specific heat capacity is an extensive quantity, so the following equation holds

$$\varepsilon_l^s c_l^s + \varepsilon_i^s c_i^s + \varepsilon_m^s c_m^s = c^s \quad (31)$$

According to Assumption 5,

$$\overline{\theta_l^s} = \overline{\theta_i^s} = \overline{\theta_m^s} = \overline{\theta^s}. \quad (32)$$

Adding Eqs. (27), (28), (29) together, and applying Eqs. (30), (31), and (32), yields the balance equation of heat for the entire s-zone:

$$y^s \omega^s c^s \frac{d}{dt} \overline{\theta_l^s} - l_{il} e_{il}^s = Q^{sB} + Q^{su} + Q^{st} + Q^{sr}, \quad (33)$$

where on the l.h.s. the first term represents the rate of change of heat storage due to variation of the temperature, and the second term represents the rate of freezing heat. The terms on the r.h.s. are REW-scale heat exchange terms of water with the groundwater reservoir, u-zone, t-zone, and r-zone, respectively, c^s is the specific heat capacity of s-zone at a constant volume, l_{il} is the latent heat of freezing.

6.4 Balance equations for unsaturated zone

6.4.1 Balance equation of mass for water phase

$$\frac{d}{dt} (\bar{\rho}_l^u \varepsilon_l^u y^u \omega^u) = e_l^{uEXT} + \sum_{L=1}^{N_K} e_l^{uL} + e_l^{us} + e_l^{ub} + e_l^{uv} + e_l^{un} + e_l^{ug} + e_{li}^u, \quad (34)$$

where the l.h.s. term represents the rate of change of water storage, the terms on the r.h.s. are various water exchange terms with the external world, neighboring REWs, s-zone, b-zone, v-zone, n-zone, g-zone, and ice phase, respectively.

From a hydrological perspective, the first two terms on the r.h.s. of Eq. (34) can be considered as subsurface and preferred flows, e_l^{us} equals $-e_l^{su}$ according to the jump condition (Reggiani et al., 1998, 1999), e_l^{ub} represents infiltration from b-zone during a storm period when positive, and capillary rise during an inter-storm period when negative which is then evaporated into the atmosphere from b-zone. Similarly, e_l^{uv} represents infiltration from v-zone during the storm period when positive, and uptake by plant roots during the inter-storm period when negative which is then transpired by vegetation, e_l^{un} and e_l^{ug} represent infiltration from snow and glacier covered zones, respectively.

6.4.2 Balance equation of mass for ice

$$\frac{d}{dt} (\bar{\rho}_i^u \varepsilon_i^u y^u \omega^u) = e_{il}^u = -e_{li}^u \quad (35)$$

6.4.3 Balance equation of momentum for water

$$\bar{\rho}_l^u \varepsilon_l^u y^u \omega^u \frac{d}{dt} \bar{v}_l^u - \bar{g}_l^u \bar{\rho}_l^u \varepsilon_l^u y^u \omega^u = T_l^{uEXT} + \sum_{L=1}^{N_K} T_l^{uL} + T_l^{us} + T_l^{ub} + T_l^{uv} + T_l^{un} + T_l^{ug} + T_{lm}^u + T_{lg}^u + T_{li}^u, \quad (36)$$

where the terms on the l.h.s. are the inertial term and weight of water, respectively. The r.h.s. terms represent various forces: the total pressure forces acting on the mantle segments in common with the external watershed boundary and with the neighboring REWs, the forces transmitted to the s-zone across the water table, to b-zone, to v-zone, to n-zone, and to g-zone, and finally, the resultant forces exchanged with the soil matrix, gas, and the ice on the water-soil matrix, water-gas, and water-ice interfaces, respectively.

Similarly, the momentum terms of T_{lm}^u and T_{li}^u can be united into one single term $T_{l(m,i)}^u$ which is denoted by T_{lm}^u unless otherwise confusion arises.

$$\bar{\rho}_l^u \varepsilon_l^u y^u \omega^u \frac{d}{dt} \bar{v}_l^u - \bar{g}_l^u \bar{\rho}_l^u \varepsilon_l^u y^u \omega^u = T_l^{uEXT} + \sum_{L=1}^{N_K} T_l^{uL} + T_l^{us} + T_l^{ub} + T_l^{uv} + T_l^{un} + T_l^{ug} + T_{lm}^u + T_{lg}^u \quad (37)$$

Similar to s-zone, we can write down the balance equations of heat for water, soil matrix, ice, and gas respectively and then add them together. In the interest of brevity, only the final results for u-zone are given.

6.4.4 Balance equation of heat for unsaturated zone

$$y^u \omega^u c^u \frac{d}{dt} \bar{\theta}^u - l_{il} e_{il}^u = Q^{us} + Q^{ub} + Q^{uv} + Q^{un} + Q^{ug}, \quad (38)$$

where on the l.h.s. the first term represents the rate of change of heat storage due to variation of the temperature, the second term accounts for the rate of freezing heat. The terms on the r.h.s. are REW-scale heat exchange terms with s-zone, b-zone, v-zone, n-zone, and g-zone, respectively.

6.5 Balance equations for bare soil zone

The bare soil zone includes the soil matrix, liquid water, and vapor. Owing to Assumption 2, vapor disperses immediately after evaporation.

6.5.1 Balance equation of mass for water phase

$$\frac{d}{dt} (\bar{\rho}_l^b y^b \omega^b) = e_l^{bT} + e_l^{bu} + e_l^{bt} + e_{lg}^b, \quad (39)$$

where the l.h.s. term represents the rate of change of depression storage, the terms on the r.h.s. account for the intensity of rainfall, water exchange rate with u-zone, with t-zone, and with the vapor phase (i.e. evaporation).

From a hydrological perspective, the exchange term, e_l^{bt} , between b-zone and t-zone, on the r.h.s. of Eq. (39) represents the runoff generated from b-zone. It is the residue after reduction of the rainfall reaching b-zone by infiltration, depression, and evaporation.

6.5.2 Balance equation of heat for bare soil zone

$$y^b \omega^b c^b \frac{d}{dt} \bar{\theta}^{surf} - l_{lg} e_{lg}^b - R_n \omega^b = Q^{bT} + Q^{bu} \quad (40)$$

where the terms on the l.h.s. are the rate of change of heat storage due to variation of temperature, the rate of latent heat transfer of vaporization, and net radiant intensity, respectively. The terms on the r.h.s. represent heat exchange rate with the atmosphere due to turbulence and with u-zone, l_{lg} is the latent heat of vaporization, and R_n is the net radiant intensity.

6.6 Balance equations for vegetated zone

6.6.1 Balance equation of mass for water phase

$$\frac{d}{dt} (\bar{\rho}_l^v \varepsilon_l^v y^v \omega^v) = e_l^{vT} + e_l^{vu} + e_l^{vt} + e_{lg}^v, \quad (41)$$

where the l.h.s. term accounts for the rate of change of water storage (i.e. canopy interception and depression storage), the

terms on the r.h.s. represent the intensity of rainfall, water exchange rate with u-zone, with t-zone, and with the vapor phase (i.e. transpiration).

6.6.2 Balance equation of heat for vegetated zone

$$y^v \omega^v c^v \frac{d}{dt} \overline{\theta^{surf}} - l_{lg} e_{lg}^v - R_n \omega^v = Q^{vT} + Q^{vu}, \quad (42)$$

where the terms on the l.h.s. are the rate of change of heat storage due to temperature variation, the rate of latent heat transfer of vaporization, and net radian intensity, respectively. The terms on the r.h.s. represent heat exchange with the atmosphere due to turbulence and with u-zone, l_{lg} is the latent heat of vaporization, and R_n is the intensity of radiation.

6.7 Balance equations for snow covered zone

6.7.1 Balance equation of mass for water phase

$$\frac{d}{dt} (\overline{\rho_l^n} \varepsilon_l^n y^n \omega^n) = e_l^{nT} + e_l^{nu} + e_l^{nt} + e_{lg}^n + e_{ln}^n, \quad (43)$$

where the l.h.s. term accounts for the rate of change of water storage, the terms on the r.h.s. represent the intensity of rainfall, water exchange rate with u-zone, with t-zone, with the vapor phase (i.e. evaporation), and with the snow phase (i.e. melting).

From a hydrological perspective, the exchange term, e_l^{nt} , between n-zone and t-zone, on the r.h.s. of Eq. (43) represents the runoff generated from n-zone. It is usually the residue after reduction of the snowmelt water by infiltration and evaporation.

6.7.2 Balance equation of mass for snow phase

$$\frac{d}{dt} (\overline{\rho_n^n} \varepsilon_n^n y^n \omega^n) = e_n^{nT} + e_{ng}^n + e_{nl}^n, \quad (44)$$

where the l.h.s. term is the rate of change of snow storage, the terms on the r.h.s. represent the intensity of snowfall, snow exchange rate with the vapor phase (i.e. sublimation) and with the water phase (i.e. melting).

6.7.3 Balance equation of heat for snow covered zone

$$y^n \omega^n c^n \frac{d}{dt} \overline{\theta^n} - l_{lg} e_{lg}^n - l_{ng} e_{ng}^n - l_{nl} e_{nl}^n - R_n \omega^n = Q^{nT} + Q^{nu}, \quad (45)$$

where the terms on the l.h.s. are the rate of change of heat storage due to temperature variation, the rate of latent heat transfer of vaporization, the rate of latent heat transfer of sublimation, the rate of heat transfer of melting, and net radian intensity, respectively. The terms on the r.h.s. represent heat exchange rate with the atmosphere due to turbulence and with u-zone, l_{lg} is the latent heat of vaporization, l_{ng} is the latent heat of sublimation, l_{nl} is the latent heat of melting, and R_n is the intensity of radiation.

6.8 Balance equations for glacier covered zone

6.8.1 Balance equation of mass for water phase

$$e_l^{gT} + e_l^{gu} + e_l^{gt} + e_{lg}^g + e_{li}^g = 0 \quad (46)$$

where the terms on the l.h.s. account for the intensity of rainfall, water exchange rate with u-zone, with t-zone, with the vapor phase (i.e. evaporation), and with the ice phase (i.e. melting or freezing). Here we omit the water storage capacity of g-zone.

From a hydrological perspective, the exchange term, e_l^{gt} , between g-zone and t-zone, on the r.h.s. of Eq. (46) represents the runoff generated from g-zone. It is the residue after reduction of the melting water by infiltration and evaporation.

6.8.2 Balance equation of mass for ice phase

$$\frac{d}{dt} (\overline{\rho_i^g} y^g \omega^g) = e_{ig}^g + e_{il}^g, \quad (47)$$

where the terms on the r.h.s. represent the rates of sublimation and freezing, respectively.

6.8.3 Balance equation of heat for glacier covered zone

$$y^g \omega^g c^g \frac{d}{dt} \overline{\theta^g} - l_{lg} e_{lg}^g - l_{ig} e_{ig}^g - l_{il} e_{il}^g - R_n \omega^g = Q^{gT} + Q^{gu}, \quad (48)$$

where the terms on the l.h.s. are the rate of change of heat storage due to variation of temperature, the rate of latent heat transfer of vaporization, the rate of latent heat transfer of sublimation, the rate of latent heat transfer of melting, and net radian intensity, respectively. The terms on the r.h.s. represent heat exchange rate with the atmosphere due to turbulence and with u-zone, l_{lg} is the latent heat of vaporization, l_{ig} is the latent heat of sublimation, l_{il} is the latent heat of melting, and R_n is the net intensity of radiation.

6.9 Balance equations for main channel reach

6.9.1 Balance equation of mass for water phase

$$\frac{d}{dt} (\overline{\rho_l^r} m^r \xi^r) = e_l^{rT} + e_l^{rEXT} + \sum_{L=1}^{N_K} e_l^{rL} + e_l^{rt} + e_l^{rs} + e_{lg}^r \quad (49)$$

where the l.h.s. term represents the rate of change of water storage, the terms on the r.h.s. are the intensity of rainfall, various water exchange rate terms with the external world, with neighboring REWs, with t-zone, with s-zone, and with the vapor phase (i.e. evaporation), respectively.

6.9.2 Balance equation of momentum for water phase

$$(\overline{\rho_l^r} m^r \xi^r) \frac{d}{dt} \overline{v_l^r} - \overline{g_l^r} \overline{\rho_l^r} m^r \xi^r$$

$$= \mathbf{T}_l^{EXT} + \sum_{L=1}^{N_K} \mathbf{T}_l^{rL} + \mathbf{T}_l^{rT} + \mathbf{T}_l^{rt} + \mathbf{T}_l^{rs}, \quad (50)$$

where the terms on the l.h.s. are the inertial term and weight of water, respectively. The r.h.s. terms represents various forces: the total pressure forces acting on the channel cross sections in common with the external watershed boundary and with the neighboring REWs, the forces transmitted to the atmosphere, to t-zone, and to s-zone, respectively.

6.9.3 Balance equation of heat for main channel reach

$$\overline{\rho_l^r} m^r \xi^r \frac{d}{dt} \overline{\theta^r} - l_g e_{lg}^r - R_n \omega^r = Q^{rT} + Q^{rs} \quad (51)$$

where the terms on the l.h.s. are the rate of change of heat storage due to variation of temperature, the rate of latent heat transfer of vaporization, and net radian intensity, respectively. The terms on the r.h.s. represent heat exchange rate with the atmosphere due to turbulence and with s-zone, l_g is the latent heat of vaporization, and R_n is the intensity of radiation.

6.10 Balance equations for sub stream network

6.10.1 Balance equation of mass for water phase

$$\frac{d}{dt} (\overline{\rho_l^t} y^t \omega^t) = e_l^{tT} + e_l^{tb} + e_l^{tv} + e_l^{tn} + e_l^{tg} + e_l^{ts} + e_l^{tr} + e_{lg}^t, \quad (52)$$

where the l.h.s. term represents the rate of change of water storage, the terms on the r.h.s. are the intensity of rainfall, various water exchange rate terms with b-zone, with v-zone, with n-zone, with g-zone, with s-zone, with r-zone, and with the vapor phase (i.e. evaporation), respectively.

6.10.2 Balance equation of momentum for water phase

$$\begin{aligned} & (\overline{\rho_l^t} y^t \omega^t) \frac{d}{dt} \overline{\mathbf{v}_l^t} - \overline{\mathbf{g}_l^t} \overline{\rho_l^t} y^t \omega^t \\ &= \mathbf{T}_l^{tT} + \mathbf{T}_l^{tb} + \mathbf{T}_l^{tv} + \mathbf{T}_l^{tn} + \mathbf{T}_l^{tg} + \mathbf{T}_l^{ts} + \mathbf{T}_l^{tr}, \end{aligned} \quad (53)$$

where the terms on the l.h.s. are the inertial term and weight of water, respectively. The r.h.s. terms represent various forces: the forces transmitted to the atmosphere, to b-zone, to v-zone, to n-zone, to g-zone, to s-zone, and to r-zone, respectively.

6.10.3 Balance equation of heat for sub stream network

$$y^t \omega^t c^t \frac{d}{dt} \overline{\theta^r} - l_g e_{lg}^t - R_n \omega^t = Q^{tT} + Q^{ts}, \quad (54)$$

where the terms on the l.h.s. are the rate of change of heat storage due to variation of temperature, the rate of latent heat transfer of vaporization, and net radian intensity, respectively. The terms on the r.h.s. represent heat exchange rate

with the atmosphere due to turbulence and with s-zone, l_g is the latent heat of vaporization, and R_n is the intensity of radiation.

7 Conclusions

The REW theory is a novel watershed hydrological modeling approach whose equations are applicable directly to the spatial scale of REW. The pioneering work by Reggiani et al. (1998, 1999) provides the unifying framework for the REW approach and the definition of REW is fundamental to it. As an initial attempt, Reggiani et al.'s definition precludes hydrological processes driven by or intimately related to energy processes, such as evaporation/transpiration, melting, freezing, and thawing, from being modeled in a physically reasonable way. After a revision of Reggiani et al.'s definition of REW, this paper derives the fundamental equations all over again, by paying particular attention to energy related processes, in order to extend the applicability of the REW approach.

In our new definition, a REW is separated into six surface sub-regions and two subsurface sub-regions. Vegetation, snow, soil ice, and glacier ice are added to the existing system including water, gas, and soil matrix. As a result, energy related processes, i.e. evaporation/transpiration occurring from various kinds of land cover and hydrological phenomena specially related with the cold region such as accumulation and depletion of snow pack and glacier, and freezing and thawing of the soil ice, can be modeled in a physically reasonable way. The sub-stream-network is separated from other sub-regions so that the sub-REW-scale runoff routing function can be represented explicitly.

The scale adaptable equations which can be applied in the watershed hydrological modeling are then formulated in a more systematic and consistent way. We first derive the general form of time-averaged conservation laws of mass, momentum, energy, and entropy at the spatial scale of REW, which is independent of any zone and any phase. After a series of assumptions aimed at watershed hydrological modeling, the interfaces, which determine the exchange terms arising in the balance equations, are simplified. The general form of conservation laws is then applied to derive the balance equations for each phase in each zone. There are in total 24 balance equations, eight of which are heat balance equations including various energy processes such as heat transfer and phase transition. For a watershed with M discrete REWs, we get finally a system of $M \times 24$ coupled equations.

Our definition and formulation procedure can be more easily applied when it is desired to include new zones and phases into the approach. This is demonstrated in Appendix B by introducing the reservoir zone in order to represent the effect of hydraulic projects on hydrological processes.

Furthermore, after introducing new assumptions or reducing existing ones, we can derive the final balance equations for other purposes by means of the general form of conservation laws. For example, we can couple the sediment movement into the current equations by ignoring the rigid assumption of soil, which is left for future research.

The subsurface heterogeneity we use is preliminary, as represented by the separation of the saturated zone and the unsaturated zone, while the layered heterogeneity along soil profile vertically is excluded. However, the additional equations could easily be coupled if we further divide the saturated zone and the unsaturated zone into several strata, which can be done in a way similar to the introduction of the reservoir zone demonstrated in Appendix B. Certainly, this will require more endeavor on additional geometric and constitutional relationships for the closure problem.

Saturation excess flow is no longer separated from infiltration excess flow in the new definition. The saturated and the unsaturated portion of the land surface which depends on the relationship between the water table and surface topography, however, can be calculated through topographic analysis such as demonstrated by Lee et al. (2005b) with the help of topographic wetness index of TOPMODEL (Beven and Kirkby, 1979).

The system of equations has a redundant number of variables for which constitutive relationships are necessary. Currently, Reggiani and Rientjes (2005) have proposed a set of closure relationships based on the exploitation of the second law, and Lee et al. (2005a, b) proposed their closure relationships based on various upscaling methods. Tian (2006) has applied Lee's procedures and formulas and Monte Carlo simulation method, and has come up with a determinate system based on the equations proposed in this paper, although these still exclude the energy balance equations. The closure relationships required by the energy related processes can be pursued by such well developed procedures and will be presented in a subsequent paper.

Appendix A

Time averaged general form of conservation laws for mass, momentum, energy and entropy

In Sect. 5.2, we obtained the general form of conservation laws, i.e. Eq. (18), based on microscopic quantities. After averaging Eq. (18) in time by integrating each term separately over the interval $(t - \Delta t, t + \Delta t)$ and dividing by $2\Delta t$ we get

$$\begin{aligned}
 & \overbrace{\frac{1}{2\Delta t} \int_{t-\Delta t}^{t+\Delta t} \left(\frac{\partial}{\partial t} \int_{V_\alpha^j} \rho_\alpha^j \psi_\alpha^j dV \right) d\tau}^{\text{temporal derivation of } \phi} \\
 & + \overbrace{\sum_{P=EXT, L, T, B, i}^{L=1..N_K, i \neq j} \frac{1}{2\Delta t} \int_{t-\Delta t}^{t+\Delta t} \int_{S_{jP}} \rho_\alpha^j \psi_\alpha^j (\mathbf{v}_\alpha^j - \mathbf{w}_\alpha^{jP}) \cdot \gamma_\alpha^j dA d\tau + \sum_{\beta \neq \alpha} \frac{1}{2\Delta t} \int_{t-\Delta t}^{t+\Delta t} \int_{S_{\alpha\beta}^j} \rho_\alpha^j \psi_\alpha^j (\mathbf{v}_\alpha^j - \mathbf{w}_{\alpha\beta}^j) \cdot dA d\tau}^{\text{spatial derivation of } \phi} \\
 & - \overbrace{\sum_{P=EXT, L, T, B, i}^{L=1..N_K, i \neq j} \frac{1}{2\Delta t} \int_{t-\Delta t}^{t+\Delta t} \int_{S_{jP}} \mathbf{i} \cdot \gamma_\alpha^j dA d\tau - \sum_{\beta \neq \alpha} \frac{1}{2\Delta t} \int_{t-\Delta t}^{t+\Delta t} \int_{S_{\alpha\beta}^j} \mathbf{i} \cdot dA d\tau}^{\text{influx}} \\
 & - \overbrace{\frac{1}{2\Delta t} \int_{t-\Delta t}^{t+\Delta t} \int_{V_\alpha^j} (\rho_\alpha^j f + G) dV d\tau}^{\text{source or sink term}} = 0
 \end{aligned} \tag{A1}$$

In the following, after presenting the definition of fluctuations and associated lemmas, we derive the time averaged form of each term in the Eq. (A1) in turn.

(1) Definition and lemmas about fluctuations of physical quantity ϕ

From the microscopic point of view, the kinetic quantities of all phases within each sub-region fluctuate around the av-

erage value which behaves similarly with turbulent flow. It is impossible and unnecessary to obtain their instantaneous value on the microscopic scale. The temporal and spatial averaging quantities are more important for watershed hydrological modeling. For this purpose, the actual movement is decomposed into two components, one is the time averaged quantity, and the other is the fluctuating quantity or residual.

This can be expressed in an equation as follows:

$$\psi_{\alpha}^j = \overline{\psi_{\alpha}^j} + \widetilde{\psi_{\alpha}^j}, \quad (\text{A2})$$

where ψ_{α}^j is the instantaneous value of the physical quantity ϕ , $\widetilde{\psi_{\alpha}^j}$ is the fluctuating value or residual, and $\overline{\psi_{\alpha}^j}$ is the time-averaged value, which is defined in Eq. (7) and Eq. (11).

About the fluctuation of physical quantity ϕ , we give the following lemmas for later use.

Lemma 1 The time averaged value of the product of two instantaneous values can be calculated by the formula

$$\overline{f_1 f_2} = \overline{f_1} \overline{f_2} + \overline{\widetilde{f_1} \widetilde{f_2}} \quad (\text{A3})$$

Lemma 2 The fluctuation value of the product of two instantaneous values can be calculated by the formula

$$\widetilde{f_1 f_2} = \overline{f_1} \widetilde{f_2} + \widetilde{f_1} \overline{f_2} + \widetilde{f_1} \widetilde{f_2} \quad (\text{A4})$$

(2) Temporal derivation term of the physical quantity ϕ

The first term on the l.h.s. of Eq. (A1) is the temporal derivative of the physical quantity ϕ . Since the order of time integration and time differentiation may be changed (Whitaker, 1981), the term can be formulated as follows, which is similar with Reggiani et al. :

$$\begin{aligned} & \frac{1}{2\Delta t} \int_{t-\Delta t}^{t+\Delta t} \left(\frac{\partial}{\partial t} \int_{V_{\alpha}^j} \rho_{\alpha}^j \psi_{\alpha}^j dV \right) d\tau \\ &= \frac{\partial}{\partial t} \left(\overline{\psi_{\alpha}^j} \overline{\rho_{\alpha}^j} \overline{\varepsilon_{\alpha}^j} \overline{y^j} \overline{\omega^j} \Sigma \right) \end{aligned} \quad (\text{A5})$$

(3) Spatial derivation term of the physical quantity ϕ

The second and third terms on the l.h.s. of Eq. (A1) are the spatial derivative terms of physical quantity ϕ , i.e. exchange rate of the physical quantity ϕ through the interface S_{α}^{jP} ($P=EXT, L, T, B, i, L=1..N_K, i \neq j$) and $S_{\alpha\beta}^j$ ($\beta \neq \alpha$), respectively. According to Eq. (A2), Eq. (A3), and the definitions of REW-scale mass exchange terms through interfaces (see Eq. (15) and Eq. (16)), the exchange rate of ϕ through S_{α}^{jP} (the second term on the l.h.s. of Eq. A1) can be formulated as follows:

$$\begin{aligned} & \frac{1}{2\Delta t} \int_{t-\Delta t}^{t+\Delta t} \int_{S_{\alpha}^{jP}} \rho_{\alpha}^j \psi_{\alpha}^j \left(\mathbf{v}_{\alpha}^j - \mathbf{w}_{\alpha}^{jP} \right) \cdot \boldsymbol{\gamma}_{\alpha}^j dA d\tau \\ &= -\overline{\psi_{\alpha}^j} e_{\alpha}^{jP} \Sigma + \frac{1}{2\Delta t} \int_{t-\Delta t}^{t+\Delta t} \int_{S_{\alpha}^{jP}} \rho_{\alpha}^j \widetilde{\psi_{\alpha}^j} \left(\mathbf{v}_{\alpha}^j - \mathbf{w}_{\alpha}^{jP} \right) \cdot \boldsymbol{\gamma}_{\alpha}^j dA d\tau \end{aligned} \quad (\text{A6})$$

Similarly, the third term on the l.h.s. of Eq. (A1) can be formulated as:

$$\begin{aligned} & \frac{1}{2\Delta t} \int_{t-\Delta t}^{t+\Delta t} \int_{S_{\alpha\beta}^j} \rho_{\alpha}^j \psi_{\alpha}^j \left(\mathbf{v}_{\alpha}^j - \mathbf{w}_{\alpha\beta}^j \right) \cdot \boldsymbol{\gamma}_{\alpha}^j dA d\tau \\ &= -\overline{\psi_{\alpha}^j} e_{\alpha\beta}^j \Sigma + \frac{1}{2\Delta t} \int_{t-\Delta t}^{t+\Delta t} \int_{S_{\alpha\beta}^j} \rho_{\alpha}^j \widetilde{\psi_{\alpha}^j} \left(\mathbf{v}_{\alpha}^j - \mathbf{w}_{\alpha\beta}^j \right) \cdot \boldsymbol{\gamma}_{\alpha}^j dA d\tau \end{aligned} \quad (\text{A7})$$

(4) Convective and non-convective terms of the physical quantity ϕ

Similar with Reggiani et al. (1998), we introduce the convective and non-convective terms in Eq. (A1). Substitution Eq. (A5), Eq. (A6), Eq. (A7), and Definition 13–18 introduced by Reggiani et al. (1998) into Eq. (A1) yields:

$$\begin{aligned} & \overbrace{\frac{\partial}{\partial t} \left(\overline{\psi_{\alpha}^j} \overline{\rho_{\alpha}^j} \overline{\varepsilon_{\alpha}^j} \overline{y^j} \overline{\omega^j} \right)}^{\text{temporal derivation term}} - \overbrace{\left(\overline{f_{\alpha}^j} \overline{\rho_{\alpha}^j} \overline{\varepsilon_{\alpha}^j} \overline{y^j} \overline{\omega^j} + \overline{G_{\alpha}^j} \overline{\varepsilon_{\alpha}^j} \overline{y^j} \overline{\omega^j} \right)}^{\text{source or sink term}} \\ & - \overbrace{\left(\sum_{P=EXT, L, T, B, i}^{L=1..N_K, i \neq j} \overline{\psi_{\alpha}^j} e_{\alpha}^{jP} + \sum_{\beta \neq \alpha} \overline{\psi_{\alpha}^j} e_{\alpha\beta}^j \right)}^{\text{convective term}} - \overbrace{\left(\sum_{P=EXT, L, T, B, i}^{L=1..N_K, i \neq j} I_{\alpha}^{jP} + \sum_{\beta \neq \alpha} I_{\alpha\beta}^j \right)}^{\text{non-convective term}} = 0 \end{aligned} \quad (\text{A8})$$

Definition 13: The non-convective term of physical quantity ϕ through interface S_{α}^{jP}

$$\begin{aligned} I_{\alpha}^{jP} &= \frac{1}{2\Delta t \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{S_{\alpha}^{jP}} \left[i - \rho_{\alpha}^j \widetilde{\psi_{\alpha}^j} \left(\mathbf{v}_{\alpha}^j - \mathbf{w}_{\alpha}^{jP} \right) \right] \cdot \boldsymbol{\gamma}_{\alpha}^j dA d\tau \\ P &= EXT, L, T, B, i, L = 1..N_K, i \neq j \end{aligned} \quad (\text{A9})$$

Definition 14: The non-convective term of physical quantity

ϕ through interface $S_{\alpha\beta}^j$

$$\begin{aligned} I_{\alpha\beta}^j &= \frac{1}{2\Delta t \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{S_{\alpha\beta}^j} \left[i - \rho_{\alpha}^j \widetilde{\psi_{\alpha}^j} \left(\mathbf{v}_{\alpha}^j - \mathbf{w}_{\alpha\beta}^j \right) \right] \cdot dA d\tau, \\ \beta &\neq \alpha \end{aligned} \quad (\text{A10})$$

Definition 15: The time-averaged generation rate of α phase in $B^j(K)$ per unit mass as:

$$\overline{f_\alpha^j} = \frac{1}{2\Delta t \overline{\rho_\alpha^j \varepsilon_\alpha^j y^j \omega^j}} \int_{t-\Delta t}^{t+\Delta t} \int_{V^j} \rho_\alpha^j f_\alpha^j \gamma_\alpha^j dV d\tau, j \neq r \quad (\text{A11})$$

Definition 16: The time-averaged generation rate of α phase in $B^r(K)$ per unit mass as:

$$\overline{f_\alpha^r} = \frac{1}{2\Delta t \overline{\rho_\alpha^r m^r \xi^r}} \int_{t-\Delta t}^{t+\Delta t} \int_{V^r} \rho_\alpha^r f_\alpha^r \gamma_\alpha^r dV d\tau \quad (\text{A12})$$

Definition 17: The time-averaged generation rate of α phase in $B^j(K)$ per unit volume as:

$$\overline{G_\alpha^j} = \frac{1}{2\Delta t \overline{\varepsilon_\alpha^j y^j \omega^j}} \int_{t-\Delta t}^{t+\Delta t} \int_{V^j} G_\alpha^j \gamma_\alpha^j dV d\tau, j \neq r \quad (\text{A13})$$

Definition 18: The time-averaged generation rate of α phase in $B^r(K)$ per unit volume as:

$$\overline{G_\alpha^r} = \frac{1}{2\Delta t m^r \xi^r} \int_{t-\Delta t}^{t+\Delta t} \int_{V^r} G_\alpha^r \gamma_\alpha^r dV d\tau \quad (\text{A14})$$

(5) General form of time averaged conservation equations

General form of mass conservation equation

The general form of mass conservation equation for α phase within j sub-region can be derived according to Table 5 such that $\psi=1, i=0, f=0$ and $G=0$ from Eq. (A8).

$$\frac{\partial}{\partial t} \left(\overline{\rho_\alpha^j \varepsilon_\alpha^j y^j \omega^j} \right) = \sum_{p=ext,l,T,B,i}^{l=1..N_K, i \neq j} e_\alpha^{jp} + \sum_{\beta \neq \alpha} e_{\alpha\beta}^j \quad (\text{A15})$$

General form of momentum conservation equation

According to the chain rule, Eq. (A8) can be rewritten as

$$\begin{aligned} & \overline{\psi_\alpha^j} \frac{\partial}{\partial t} \left(\overline{\rho_\alpha^j \varepsilon_\alpha^j y^j \omega^j} \right) + \left(\overline{\rho_\alpha^j \varepsilon_\alpha^j y^j \omega^j} \right) \frac{\partial}{\partial t} \left(\overline{\psi_\alpha^j} \right) \\ &= \overline{f_\alpha^j} \overline{\rho_\alpha^j \varepsilon_\alpha^j y^j \omega^j} + \overline{G_\alpha^j} \overline{\varepsilon_\alpha^j y^j \omega^j} + \sum_{P=EXT,L,T,B,i}^{L=1..N_K, i \neq j} \overline{\psi_\alpha^j} e_\alpha^{jP} + \sum_{\beta \neq \alpha} \overline{\psi_\alpha^j} e_{\alpha\beta}^j + \sum_{P=EXT,L,T,B,i}^{L=1..N_K, i \neq j} I_\alpha^{jP} + \sum_{\beta \neq \alpha} I_{\alpha\beta}^j \end{aligned} \quad (\text{A16})$$

Multiplication of the mass conservation Eq. (A15) by the $\overline{\psi_\alpha^j}$ and subsequent subtraction from Eq. (A16) gives the general

form of time averaged conservation equations of momentum, energy, and entropy as follows:

$$\left(\overline{\rho_\alpha^j \varepsilon_\alpha^j y^j \omega^j} \right) \frac{\partial}{\partial t} \left(\overline{\psi_\alpha^j} \right) = \overline{f_\alpha^j} \overline{\rho_\alpha^j \varepsilon_\alpha^j y^j \omega^j} + \overline{G_\alpha^j} \overline{\varepsilon_\alpha^j y^j \omega^j} + \sum_{P=EXT,L,T,B,i}^{L=1..N_K, i \neq j} I_\alpha^{jP} + \sum_{\beta \neq \alpha} I_{\alpha\beta}^j \quad (\text{A17})$$

Therefore, the general form of momentum conservation equation for α phase within j sub-region can be derived according to Table 5 such that $\psi=\mathbf{v}, i=\mathbf{t}, f=\mathbf{g}$ and $G=0$ from

Eq. (A32) (for clarity, non-convective momentum is denoted by the symbol \mathbf{T}):

$$\left(\overline{\rho_\alpha^j \varepsilon_\alpha^j y^j \omega^j} \right) \frac{d}{dt} \left(\overline{\mathbf{v}_\alpha^j} \right) = \overline{\mathbf{g}_\alpha^j} \overline{\rho_\alpha^j \varepsilon_\alpha^j y^j \omega^j} + \sum_{P=EXT,L,T,B,i}^{L=1..N_K, i \neq j} \mathbf{T}_\alpha^{jP} + \sum_{\beta \neq \alpha} \mathbf{T}_{\alpha\beta}^j \quad (\text{A18})$$

where:

$$\mathbf{T}_\alpha^{jP} = \frac{1}{2\Delta t \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{S_{jP}} \left[\mathbf{t} - \rho_\alpha^j \tilde{\mathbf{v}}_\alpha^j \left(\mathbf{v}_\alpha^j - \mathbf{w}_{\alpha\beta}^{jP} \right) \right] \cdot \gamma_\alpha^j dA d\tau \quad (\text{A19})$$

$P = EXT, L, T, B, i, L = 1..N_K, i \neq j$

$$\mathbf{T}_{\alpha\beta}^j = \frac{1}{2\Delta t \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{S_{\alpha\beta}^j} \left[\mathbf{t} - \rho_\alpha^j \tilde{\mathbf{v}}_\alpha^j \left(\mathbf{v}_\alpha^j - \mathbf{w}_{\alpha\beta}^j \right) \right] \cdot dA d\tau \quad (\text{A20})$$

General form of energy conservation equation

The general form of energy conservation equation for α phase within j sub-region can be derived according to Table 5 such that $\psi=E+1/2v^2, i=\mathbf{t} \cdot \mathbf{v} + q, f=h+\mathbf{g} \cdot \mathbf{v}$ and

$G=0$ from Eq. (A8):

$$\begin{aligned} & \left(\overline{\rho_\alpha^j \varepsilon_\alpha^j y^j \omega^j} \right) \frac{\partial}{\partial t} \left(\overline{E+1/2v_\alpha^{j2}} \right) \\ &= \overline{(h_\alpha^j + \mathbf{g}_\alpha^j \cdot \mathbf{v}_\alpha^j)} \overline{\rho_\alpha^j \varepsilon_\alpha^j y^j \omega^j} \\ &+ \sum_{P=EXT,L,T,B,i}^{L=1..N_K, i \neq j} I_\alpha^{jP} + \sum_{\beta \neq \alpha} I_{\alpha\beta}^j \end{aligned} \quad (\text{A21})$$

where

$$I_{\alpha}^{jP} = \frac{1}{2\Delta t \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_S \left[\mathbf{t} \cdot \mathbf{v}_{\alpha}^j + q - \rho_{\alpha}^j \left(\overline{E_{\alpha}^j + (v_{\alpha}^j)^2 / 2} \right) (\mathbf{v}_{\alpha}^j - \mathbf{w}_{\alpha}^{jP}) \right] \cdot \gamma_{\alpha}^j dA d\tau$$

$$I_{\alpha\beta}^j = \frac{1}{2\Delta t \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{S_{\alpha\beta}^j} \left[\mathbf{t} \cdot \mathbf{v}_{\alpha}^j - \rho_{\alpha}^j \left(\overline{E_{\alpha}^j + (v_{\alpha}^j)^2 / 2} \right) (\mathbf{v}_{\alpha}^j - \mathbf{w}_{\alpha\beta}^j) \right] \cdot dA d\tau, \beta \neq \alpha$$

The l.h.s. term in Eq. (A21) can be formulated according to Lemmas 1 as:

$$\left(\overline{\rho_{\alpha}^j \varepsilon_{\alpha}^j y^j \omega^j} \right) \frac{\partial}{\partial t} \left(\overline{E + 1/2 v_{\alpha}^{j2}} \right)$$

$$= \left(\overline{\rho_{\alpha}^j \varepsilon_{\alpha}^j y^j \omega^j} \right) \frac{\partial}{\partial t} \left(\overline{E} + \frac{1}{2} \overline{(v_{\alpha}^j)^2} + \frac{1}{2} \overline{(v_{\alpha}^j)^2} \right) \quad (\text{A22})$$

In the interest of brevity, we introduce the following definition.

Definition 19: The time averaged value of the generalized internal energy of B_{α}^j is defined as:

$$\widehat{E_{\alpha}^j} = \overline{E_{\alpha}^j} + \overline{v_{\alpha}^{j2}} / 2 \quad (\text{A23})$$

Definition 20: The fluctuation value of the generalized internal energy of B_{α}^j is defined as:

$$\overline{E_{\alpha}^j} = E_{\alpha}^j - \widehat{E_{\alpha}^j} = \widetilde{E_{\alpha}^j} - \overline{v_{\alpha}^{j2}} / 2 \quad (\text{A24})$$

Definition 21: The time averaged value of the generalized external energy of B_{α}^j :

$$\widehat{h_{\alpha}^j} = \overline{h_{\alpha}^j} + \overline{\mathbf{g}_{\alpha}^j \cdot \mathbf{v}_{\alpha}^j} \quad (\text{A25})$$

Therefore, the l.h.s. term in Eq. (A21) can be rewritten according to Eq. (A22) and Eq. (A23) as

$$\left(\overline{\rho_{\alpha}^j \varepsilon_{\alpha}^j y^j \omega^j} \right) \frac{\partial}{\partial t} \left(\overline{E + 1/2 v_{\alpha}^{j2}} \right)$$

$$= \left(\overline{\rho_{\alpha}^j \varepsilon_{\alpha}^j y^j \omega^j} \right) \frac{\partial}{\partial t} \left(\widehat{E} + \frac{1}{2} \overline{(v_{\alpha}^j)^2} \right). \quad (\text{A26})$$

The first term on the r.h.s. of Eq. (A21) can be formulated according to Lemma 1 and Eq. (A25) as:

$$\left(\overline{h_{\alpha}^j + \mathbf{g}_{\alpha}^j \cdot \mathbf{v}_{\alpha}^j} \right) \overline{\rho_{\alpha}^j \varepsilon_{\alpha}^j y^j \omega^j}$$

$$= \left(\widehat{h_{\alpha}^j} + \overline{\mathbf{g}_{\alpha}^j \cdot \mathbf{v}_{\alpha}^j} \right) \overline{\rho_{\alpha}^j \varepsilon_{\alpha}^j y^j \omega^j} \quad (\text{A27})$$

After introducing of Definition 22, the non-convective term across the interface S^{jP} can be formulated according to Lemma 2, Eq. (A24), Eq. (A2), and Eq. (A19) as:

$$I_{\alpha}^{jP} = \mathbf{T}_{\alpha}^{jP} \cdot \overline{\mathbf{v}_{\alpha}^j} + Q_{\alpha}^{jP} \quad (\text{A28})$$

Definition 22: The generalized energy exchange term across the interface S^{jP} :

$$Q_{\alpha}^{jP} = \frac{1}{2\Delta t \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{S^{jP}} \left[q + \mathbf{t} \cdot \widetilde{\mathbf{v}_{\alpha}^j} - \rho_{\alpha}^j \left(\overline{E_{\alpha}^j} + \frac{1}{2} \overline{v_{\alpha}^{j2}} \right) (\mathbf{v}_{\alpha}^j - \mathbf{w}_{\alpha}^{jP}) \right] \cdot \gamma_{\alpha}^j dA d\tau. \quad (\text{A29})$$

Similarly, by introducing Definition 23, the non-convective term across the interface $S_{\alpha\beta}^j$ can be rewritten as

$$I_{\alpha\beta}^j = \mathbf{T}_{\alpha\beta}^j \cdot \overline{\mathbf{v}_{\alpha}^j} + Q_{\alpha\beta}^j \quad (\text{A30})$$

Definition 23: The generalized energy exchange term across the interface $S_{\alpha\beta}^j$:

$$Q_{\alpha\beta}^j = \frac{1}{2\Delta t \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{S_{\alpha\beta}^j} \left[q + \mathbf{t} \cdot \widetilde{\mathbf{v}_{\alpha}^j} - \rho_{\alpha}^j \left(\overline{E_{\alpha}^j} + \frac{1}{2} \overline{v_{\alpha}^{j2}} \right) (\mathbf{v}_{\alpha}^j - \mathbf{w}_{\alpha\beta}^j) \right] \cdot dA d\tau \quad (\text{A31})$$

Substitution of Eq. (A26), Eq. (A27), Eq. (A28), and Eq. (A30) into Eq. (A21) yields the general form of averaged energy conservation equation.

$$\begin{aligned} & \left(\overline{\rho_\alpha^j \varepsilon_\alpha^j y^j \omega^j} \right) \frac{d}{dt} \left(\overline{E_\alpha^j} + \overline{v_\alpha^j}^2 / 2 \right) \\ &= \left(\overline{h_\alpha^j} + \overline{\mathbf{g}_\alpha^j \cdot \mathbf{v}_\alpha^j} \right) \overline{\rho_\alpha^j \varepsilon_\alpha^j y^j \omega^j} + \sum_{P=EXT, L, T, B, i}^{L=1..N_K, i \neq j} \left(\overline{\mathbf{T}_\alpha^{jP} \cdot \mathbf{v}_\alpha^j} + \overline{Q_\alpha^{jP}} \right) \\ &+ \sum_{\beta \neq \alpha} \left(\overline{\mathbf{T}_{\alpha\beta}^j \cdot \mathbf{v}_\alpha^j} + \overline{Q_{\alpha\beta}^j} \right). \end{aligned} \quad (\text{A32})$$

After dot product of the velocity vector $\overline{\mathbf{v}_\alpha^j}$ with the momentum balance Eq. (A18) we will get the mechanical energy conservation equation, similar with Reggiani et al. (1998):

$$\begin{aligned} & \left(\overline{\rho_\alpha^j \varepsilon_\alpha^j y^j \omega^j} \right) \frac{d}{dt} \left(\overline{v_\alpha^j}^2 / 2 \right) \\ &= \overline{\mathbf{g}_\alpha^j \cdot \mathbf{v}_\alpha^j} \overline{\rho_\alpha^j \varepsilon_\alpha^j y^j \omega^j} + \sum_{P=EXT, L, T, B, i}^{L=1..N_K, i \neq j} \left(\overline{\mathbf{T}_\alpha^{jP} \cdot \mathbf{v}_\alpha^j} \right) \\ &+ \sum_{\beta \neq \alpha} \left(\overline{\mathbf{T}_{\alpha\beta}^j \cdot \mathbf{v}_\alpha^j} \right). \end{aligned} \quad (\text{A33})$$

And the internal energy conservation equation is obtained from Eq. (A32), after subtraction of the mechanical energy conservation Eq. (A33):

$$\begin{aligned} & \left(\overline{\rho_\alpha^j \varepsilon_\alpha^j y^j \omega^j} \right) \frac{d\overline{E_\alpha^j}}{dt} = \overline{h_\alpha^j \rho_\alpha^j \varepsilon_\alpha^j y^j \omega^j} \\ &+ \sum_{P=EXT, L, T, B, i}^{L=1..N_K, i \neq j} \overline{Q_\alpha^{jP}} \\ &+ \sum_{\beta \neq \alpha} \overline{Q_{\alpha\beta}^j}. \end{aligned} \quad (\text{A34})$$

Furthermore, after ignoring any additional item caused by the fluctuation of velocity and internal energy in Eq. (A34), the balance equation of heat is derived:

$$\begin{aligned} & \left(\varepsilon_\alpha^j y^j \omega^j c_\alpha^j \right) \frac{d\overline{\theta_\alpha^j}}{dt} = \overline{h_\alpha^j \rho_\alpha^j \varepsilon_\alpha^j y^j \omega^j} \\ &+ \sum_{P=EXT, L, T, B, i}^{L=1..N_K, i \neq j} \overline{Q_\alpha^{jP}} \\ &+ \sum_{\beta \neq \alpha} \overline{Q_{\alpha\beta}^j}, \end{aligned} \quad (\text{A35})$$

where c_α^j represents the specific heat capacity of α phase at constant volume averaged over j zone, $\overline{\theta_\alpha^j}$ represents the temperature of α phase averaged over j zone, $\overline{Q_\alpha^{jP}}$ represents the heat transferred from α phase in P zone to that in j zone,

$\overline{Q_{\alpha\beta}^j}$ represents the heat transferred from β phase to α phase in j zone, and

$$\overline{Q_\alpha^{jP}} = \frac{1}{2\Delta t \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{S_{jP}} q \cdot \gamma_\alpha^j dA d\tau \quad (\text{A36})$$

$$\overline{Q_{\alpha\beta}^j} = \frac{1}{2\Delta t \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{S_{\alpha\beta}^j} q \cdot dA d\tau \quad (\text{A37})$$

For convenience, $\overline{Q_\alpha^{jP}}$ and $\overline{Q_{\alpha\beta}^j}$ are still denoted by Q_α^{jP} and $Q_{\alpha\beta}^j$ unless otherwise confusion arises. The final result of heat balance equation is as following:

$$\begin{aligned} & \left(\varepsilon_\alpha^j y^j \omega^j c_\alpha^j \right) \frac{d\overline{\theta_\alpha^j}}{dt} = \overline{h_\alpha^j \rho_\alpha^j \varepsilon_\alpha^j y^j \omega^j} \\ &+ \sum_{P=EXT, L, T, B, i}^{L=1..N_K, i \neq j} Q_\alpha^{jP} \\ &+ \sum_{\beta \neq \alpha} Q_{\alpha\beta}^j \end{aligned} \quad (\text{A38})$$

General form of entropy conservation equation

The general form of the entropy conservation equation for α phase within j sub-region can be derived according to Table 5 such that $\psi=\eta$, $i=j$, $f=b$ and $G=L$ from Eq. (A17) (for clarity, non-convective entropy is denoted by the symbol F):

$$\begin{aligned} & \left(\overline{\rho_\alpha^j \varepsilon_\alpha^j y^j \omega^j} \right) \frac{d\overline{\eta_\alpha^j}}{dt} = \overline{b_\alpha^j \rho_\alpha^j \varepsilon_\alpha^j y^j \omega^j} \\ &+ \overline{L_\alpha^j \varepsilon_\alpha^j y^j \omega^j} + \sum_{P=EXT, L, T, B, i}^{L=1..N_K, i \neq j} \overline{F_\alpha^{jP}} \\ &+ \sum_{\beta \neq \alpha} \overline{F_{\alpha\beta}^j} \end{aligned} \quad (\text{A39})$$

where:

$$\begin{aligned} & \overline{F_\alpha^{jP}} = \frac{1}{2\Delta t \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{S_{jP}} \left[j - \rho_\alpha^j \tilde{\eta}_\alpha^j \left(\mathbf{v}_\alpha^j - \mathbf{w}_\alpha^{jP} \right) \right] \cdot \gamma_\alpha^j dA d\tau \\ &P = EXT, L, T, B, i, L = 1..N_K, i \neq j \end{aligned} \quad (\text{A40})$$

$$\begin{aligned} & \overline{F_{\alpha\beta}^j} = \frac{1}{2\Delta t \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{S_{\alpha\beta}^j} \left[j - \rho_\alpha^j \tilde{\eta}_\alpha^j \left(\mathbf{v}_\alpha^j - \mathbf{w}_{\alpha\beta}^j \right) \right] \cdot dA d\tau, \\ &\beta \neq \alpha \end{aligned} \quad (\text{A41})$$

Appendix B

The revised and supplementary balance equations after introducing the reservoir zone into the existing REW system

In this paper, a REW with six surface sub-regions and two subsurface sub-regions is defined and the corresponding time-averaged balance equations are derived. Such definition

Table B1. The additional interfaces after introducing the reservoir zone.

No	Sub-region	Additional interfaces
1	s-zone	S^{so}
2	u-zone	S^{uo}
3	r-zone	$S^{ro} = S^{ro-u} + S^{ro-d}$
4	t-zone	S^{to}
5	o-zone	$S^{oT}, S^{os}, S^{ou}, S^{or}, S^{ot}, S_{lp}^o$

will meet the requirements of most watershed hydrological modeling. However, it is necessary to add new sub-regions into the existing REW system in some special situations. For example, the additional reservoir zone is needed in order to incorporate the regulation function of hydraulic projects. The newly defined compositive zone of two or more basic types of land cover such as snow and vegetation, or different vegetation zones could be needed for detailed simulation. Also, for consideration of subsurface heterogeneity, one could divide the unsaturated zone or saturated zone into several layers and hence introduce more zones. In this Appendix, we will take the reservoir for example to demonstrate how to derive the revised and supplementary balance equations owing to the introduction of new zones into the existing REW system.

(1) Introducing the reservoir zone into the REW definition

For incorporating the effect of hydraulic projects on hydrological processes, the reservoir zone, shortly named as o-zone, is separated from the sub-stream-network zone in the REW definition presented in Sect.3. The surface layer of REW is, then, composed of seven sub-regions. On the spatial side, the seven sub-regions constitute a complete cover of the land surface in the horizontal direction. In the vertical direction, it can be considered that o-zone lies above the saturated zone.

The reservoir zone receives water from upstream main channel reach and t-zone, and releases water into the downstream main channel reach which is regulated according to the different purposes such as flood prevention, water supply, power generation, and so on. It also exchanges water with s-zone vertically and supplies water for u-zone laterally in the subsurface layer. Similar with t-zone, the substances contained within o-zone are water and vapor.

(2) The additional interfaces after introducing the reservoir zone

Following the assumptions introduced in Sect. 6.1 and the function of o-zone discussed above, the existing interfaces summarized in Table 6 should be supplemented by the newly introduced interfaces delimiting o-zone from s-zone, u-zone, t-zone, and r-zone, which are denoted in turn by S^{so} , S^{uo} , S^{to} , and S^{ro} . Moreover, the interface between o-zone and

r-zone, S^{ro} , can be further divided into two sections, i.e. upstream section and downstream section, which are denoted by S^{ro-u} and S^{ro-d} , respectively. These additional interfaces are summarized in Table B1.

(3) The revised and newly introduced balance equations

The general form of the conservation laws developed in Sect. 5 holds true in spite of the introduction of the reservoir zone. However, the pragmatic form of balance equations for the existing sub-regions listed in Sect. 6.3–6.10 should be revised, and the new balance equations of mass, momentum, and heat should be introduced following the procedure proposed in Sect. 6. The existing equations should be revised by adding the additional exchange terms of mass, momentum, and heat according to the additional interfaces summarized in Table B1. The final results are referred in Table B2.

The newly introduced equations for o-zone are listed below.

Balance equation of mass for water phase:

$$\frac{d}{dt} (\bar{\rho}_l^o y^o \omega^o) = e_l^{oT} + e_l^{os} + e_l^{ou} + e_l^{or-u} + e_l^{or-d} + e_l^{ot} + e_{lg}^o \quad (\text{A42})$$

where the l.h.s. term represents the rate of change of water storage, the terms on the r.h.s. are the intensity of rainfall, various water exchange rate terms with s-zone, with u-zone, with upstream main channel reach, with downstream main channel reach, with t-zone, and with the vapor phase (i.e. evaporation), respectively.

Balance equation of momentum for water phase:

$$\begin{aligned} \bar{\rho}_l^o y^o \omega^o \frac{d}{dt} \bar{v}_l^o - \bar{\mathbf{g}}_l^o \bar{\rho}_l^o y^o \omega^o \\ = \mathbf{T}_l^{oT} + \mathbf{T}_l^{os} + \mathbf{T}_l^{ou} + \mathbf{T}_l^{or-u} + \mathbf{T}_l^{or-d} + \mathbf{T}_l^{ot} \end{aligned} \quad (\text{A43})$$

where the terms on the l.h.s. are the inertial term and weight of water, respectively. The r.h.s. terms represent various forces: the forces transmitted to the atmosphere, to s-zone, to u-zone, to upstream main channel, to downstream main channel, and to t-zone, respectively.

Balance equation of heat for reservoir zone:

$$y^o \omega^o c^o \frac{d}{dt} \bar{\theta}^o - l_{lg} e_{lg}^o - R_n \omega^o = Q^{tT} + Q^{os} \quad (\text{A44})$$

where the terms on the l.h.s. are the rate of change of heat storage due to variation of temperature, the rate of latent

Table B2. The revised equations after introducing the reservoir zone.

No	Sub-region	Physical quantity	Revised equation	Original equation
1	s-zone	mass	$\frac{d}{dt} (\bar{\rho}_l^s \varepsilon_l^s y^s \omega^s) = e_l^{sEXT} + \sum_{L=1}^{N_K} e_l^{sL} + e_l^{sB} + e_l^{su} + e_l^{st} + e_l^{sr} + e_l^{so} + e_{li}^s$	Eq. (23)
2		momentum	$\bar{\rho}_l^s \varepsilon_l^s y^s \omega^s \frac{d}{dt} \bar{\mathbf{v}}_l^s - \bar{\mathbf{g}}_l^s \bar{\rho}_l^s \varepsilon_l^s y^s \omega^s = \mathbf{T}_l^{sEXT} + \sum_{L=1}^{N_K} \mathbf{T}_l^{sL} + \mathbf{T}_l^{sB} + \mathbf{T}_l^{su} + \mathbf{T}_l^{st} + \mathbf{T}_l^{sr} + \mathbf{T}_l^{so} + \mathbf{T}_{lm}^s + \mathbf{T}_{li}^s$	Eq. (25)
3		heat	$y^s \omega^s c^s \frac{d}{dt} \bar{\theta}_l^s - l_{il} \varepsilon_{il}^s = Q^{sB} + Q^{st} + Q^{sr} + Q^{so}$	Eq. (33)
4	u-zone	mass	$\frac{d}{dt} (\bar{\rho}_l^u \varepsilon_l^u y^u \omega^u) = e_l^{uEXT} + \sum_{L=1}^{N_K} e_l^{uL} + e_l^{uo} + e_l^{us} + e_l^{ub} + e_l^{uv} + e_l^{un} + e_l^{ug} + e_{li}^u$	Eq. (34)
5		momentum	$\bar{\rho}_l^u \varepsilon_l^u y^u \omega^u \frac{d}{dt} \bar{\mathbf{v}}_l^u - \bar{\mathbf{g}}_l^u \bar{\rho}_l^u \varepsilon_l^u y^u \omega^u = \mathbf{T}_l^{uEXT} + \sum_{L=1}^{N_K} \mathbf{T}_l^{uL} + \mathbf{T}_l^{uo} + \mathbf{T}_l^{us} + \mathbf{T}_l^{ub} + \mathbf{T}_l^{uv} + \mathbf{T}_l^{un} + \mathbf{T}_l^{ug} + \mathbf{T}_{lm}^u + \mathbf{T}_{lg}^u + \mathbf{T}_{li}^u$	Eq. (36)
6	r-zone	Mass	$\frac{d}{dt} (\bar{\rho}_l^r m^r \xi^r) = e_l^{rT} + e_l^{rEXT} + \sum_{L=1}^{N_K} e_l^{rL} + e_l^{rt} + e_l^{rs} + e_l^{ro,u} + e_l^{ro,d} + e_{lg}^r$	Eq. (49)
7		momentum	$(\bar{\rho}_l^r m^r \xi^r) \frac{d}{dt} \bar{\mathbf{v}}_l^r - \bar{\mathbf{g}}_l^r \bar{\rho}_l^r m^r \xi^r = \mathbf{T}_l^{rEXT} + \sum_{L=1}^{N_K} \mathbf{T}_l^{rL} + \mathbf{T}_l^{rT} + \mathbf{T}_l^{rt} + \mathbf{T}_l^{rs} + \mathbf{T}_l^{ro,u} + \mathbf{T}_l^{ro,d}$	Eq. (50)
4	t-zone	Mass	$\frac{d}{dt} (\bar{\rho}_l^t y^t \omega^t) = e_l^{tT} + e_l^{tb} + e_l^{tv} + e_l^{tn} + e_l^{tg} + e_l^{tr} + e_l^{to} + e_{lg}^t$	Eq. (52)
5		momentum	$(\bar{\rho}_l^t y^t \omega^t) \frac{d}{dt} \bar{\mathbf{v}}_l^t - \bar{\mathbf{g}}_l^t \bar{\rho}_l^t y^t \omega^t = \mathbf{T}_l^{tT} + \mathbf{T}_l^{tb} + \mathbf{T}_l^{tv} + \mathbf{T}_l^{tn} + \mathbf{T}_l^{tg} + \mathbf{T}_l^{tr} + \mathbf{T}_l^{to}$	Eq. (53)

Note: the balance equations of heat for u-zone, r-zone, and t-zone keep the original form due to the Assumption 6.

heat transfer of vaporization, and net radian intensity, respectively. The terms on the r.h.s. represent heat exchange rate with the atmosphere due to turbulence and with s-zone, l_{lg}

is the latent heat of vaporization, and R_n is the intensity of radiation.

Nomenclature

Latin symbols

b	the entropy supply from the external world	
B	the body of a continuum	
$B(K)$	the K th REW	
$B^j(K)$	the body of j sub-region continuum divided from $B(K)$, $j \in \{e e = u, s, r, t, b, v, n, g\}$	
$B_\alpha^j(K)$	the body of α phase in j sub-region divided from $B(K)$, $j \in \{e e = u, s, r, t, b, v, n, g\}, \alpha \in \{\zeta \zeta = m, l, a, p, i, n, v\}$	
c^j	the specific heat capacity of j zone at a constant volume	$[L^2 T^{-2} \Theta^{-1}]$
c_α^j	the specific heat capacity of α phase in j zone at a constant volume	$[L^2 T^{-2} \Theta^{-1}]$
$C(K)$	the contour of $S^T(K)$	
$dS^{jEXT}(K)$	the differential area vector for $S^{jEXT}(K)$	$[L^2]$
$dS^{jL}(K)$	the differential area vector for $S^{jL}(K)$	$[L^2]$
$dS^{jT}(K)$	the differential area vector for $S^{jT}(K)$	$[L^2]$
$dS^{jB}(K)$	the differential area vector for $S^{jB}(K)$	$[L^2]$
$dS^{ji}(K)$	the differential area vector for $S^{ji}(K)$	$[L^2]$
$dS_{\alpha\beta}^j(K)$	the differential area vector for $S_{\alpha\beta}^j(K)$	$[L^2]$
e_α^{jP}	the net flux of α phase through S^{jP}	$ML^{-2}T^{-1}$
$e_{\alpha\beta}^j$	the phase transition rate between α phase and β phase	$ML^{-2}T^{-1}$
E	the microscopic internal energy per unit mass	$[L^2 T^{-2}]$
\widehat{E}_α^j	the time-averaged value of the generalized internal energy of B_α^j	$[MT^{-2}]$
\widehat{E}_α^j	the fluctuation value of the generalized internal energy of B_α^j	$[MT^{-2}]$
f	the source or sink term per unit mass	

$\overline{f_\alpha^j}$	the time-averaged generation rate of α phase in j zone per unit mass	
\mathbf{g}	the gravity accelerator vector	$[LT^{-2}]$
G	the source or sink term per unit volume	
$\overline{G_\alpha^j}$	the time-averaged generation rate of α phase in j zone per unit volume	
h	the supply of internal energy from outside world	$[MT^{-3}]$
$\widehat{h_\alpha^j}$	the time-averaged value of the generalized external energy of B_α^j	$[MT^{-3}]$
\mathbf{i}	the diffusion flux	
I_α^{jP}	the non-convective term of physical quantity ϕ through the interface S_α^{jP}	
$I_{\alpha\beta}^j$	the non-convective term of physical quantity ϕ through the interface $S_{\alpha\beta}^j$	
\mathbf{j}	the non-convective flux of entropy	
K	indicate the K th REW	
L	the entropy production within the continuum	
l^r	the instantaneous length of the main channel reach	$[L]$
m^r	the time-averaged cross section area of the main channel reach	$[L^2]$
M	the number of discrete REWs in a watershed	
N_K	the number of REWs neighboring $B(K)$	
\mathbf{q}	the microscopic heat flux vector	$[MT^{-3}]$
Q_α^{jP}	the generalized energy exchange term across the interface S_α^{jP}	$[MT^{-3}]$
$Q_{\alpha\beta}^j$	the generalized energy exchange term across the interface $S_{\alpha\beta}^j$	$[MT^{-3}]$
$\underline{Q_\alpha^{jP}}$	the heat transferred from α phase in P zone to that in j zone	$[MT^{-3}]$
$\underline{Q_{\alpha\beta}^j}$	the heat transferred from β phase to α phase in j zone	$[MT^{-3}]$
R_n	the intensity of radiation	$[MT^{-3}]$
$S(K)$	the surface of $B(K)$	$[L^2]$
$S^{EXT}(K)$	the segment formed by the interfaces between $B(K)$ and the external world	$[L^2]$
$S^L(K)$	the segment formed by the interfaces between $B(K)$ and $B(L)$	$[L^2]$
$S^T(K)$	the top surface formed by the land surface covering $B(K)$	$[L^2]$
$S^B(K)$	the bottom surface of $B(K)$, can be either the impermeable strata or a hypothetical plane at a given depth reaching into the groundwater reservoir, or a combination of the two	$[L^2]$
$S^{jEXT}(K)$	the interface between $B^j(K)$ and the external world	$[L^2]$
$S^{jL}(K)$	the interface between $B^j(K)$ and $B(L)$ ($L = 1..N_K$)	$[L^2]$
$S^{jT}(K)$	the interface between $B^j(K)$ and the atmosphere	$[L^2]$
$S^{jB}(K)$	the interface between $B^j(K)$ and the impermeable strata or the groundwater reservoir	$[L^2]$
$S^{ji}(K)$	the interface between $B^j(K)$ and other sub-regions within the same REW, $B^i(K)$ ($i \neq j$)	$[L^2]$
$S_{\alpha\beta}^j(K)$	the phase interface between $B_\alpha^j(K)$ and $B_\beta^j(K)$	$[L^2]$
$S^{jP}(K)$	the area vector of interface $S_\alpha^{jP}(K)$	$[L^2]$
\mathbf{t}	the microscopic stress tensor	$[ML^{-1}T^{-2}]$
\mathbf{T}_α^{jP}	the non-convective momentum through the interface S_α^{jP}	$[MLT^{-2}]$
\mathbf{v}	velocity of the a continuum	$[LT^{-1}]$
$V(K)$	the space occupied by all the substances contained in $B(K)$	$[L^3]$
$V^j(K)$	the volume occupied by $B^j(K)$	$[L^3]$
$V_\alpha^j(K)$	the volume occupied by $B_\alpha^j(K)$	$[L^3]$
\mathbf{w}	velocity of a continuum interface	$[LT^{-1}]$
y^j	the time-averaged thickness of B^j	$[L]$

Greek symbols

Δt	time interval for equation averaging	[T]
ε_{α}^j	the time-averaged volume of B_{α}^j relative to V^j	
ε_l^u	water content of the unsaturated zone	
ε_l^s	water content of the saturated zone	
ϕ	physical quantity	
γ_{α}^j	the phase distribution function on α phase in j zone	
η	the microscopic entropy per unit mass	
κ_{α}^{jP}	the fraction of heat exchange term Q^{jP} absorbed by α phase	
λ_{α}	the fraction of fusion heat absorbed by α phase	
$\overline{\theta_{surf}}$	the averaged temperature of the surface sub-regions	[Θ]
$\overline{\theta_{\alpha}^j}$	the temperature of α phase in j zone	[Θ]
$\overline{\rho_{\alpha}^j}$	the time-averaged density of B_{α}^j	[ML^{-3}]
ρ_{α}^j	the density of α phase at the differential volume dV in V_{α}^j space	[ML^{-3}]
$\Sigma(K)$	the horizontal projected area of $B(K)$	[L^2]
$\Sigma^j(K)$	the horizontal projected area of $B^j(K)$	[L^2]
ω^j	the time-averaged horizontal projected area of B^j	[L^2]
ξ^r	the time-averaged length of the main channel reach relative to Σ	[L^{-1}]
ψ_{α}^j	the instantaneous value of physical quantity ϕ possessed by B_{α}^j relative to the mass of B_{α}^j	
$\overline{\psi_{\alpha}^j}$	the time-averaged physical quantity ϕ possessed by B_{α}^j relative to the mass of B_{α}^j	
$\widetilde{\psi_{\alpha}^j}$	the fluctuant value of physical quantity ϕ possessed by B_{α}^j relative to the mass of B_{α}^j	

Subscripts and superscripts

B	superscript indicating the impermeable strata or groundwater reservoir
EXT	superscript indicating the external world
i, j	superscripts indicating sub-region, can be u (unsaturated zone), s(saturated zone), r (main channel reach), t (sub-stream-network), b (bare soil zone), v (vegetated zone), n (snow covered zone), g (glacier covered zone), o (reservoir zone)
L	superscript indicating the neighboring REW, $L=1..N_K$
P	superscript indicating the wildcard indicating $EXT, L, T, B, i, L=1..N_K$
T	superscript indicating the atmosphere
α, β	subscripts indicating the phase, can be m (soil matrix), l (liquid water), a (gaseous phase), p (vapor), i (ice), n (snow), and v (vegetation)

Note: M is the dimension of mass, L is the dimension of length, T is the dimension of time, and Θ is the dimension of temperature.

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